Supporting Materials

Extension of the Polarizable Charge Equilibration Model to Higher Oxidation States with Applications to Ge, As, Se, Br, Sn, Sb, Te, I, Pb, Bi, Po, and At Elements

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1. Parameter Set for PQEq2

Table S1: The electronegativity χ, idempotential J, shell charge Q_c, atomic covalent radius $R_c=R_s$, and spring force constant K_s for PQEq2.

Atom	χ (eV)	J (eV)	Q_c	$R_c=R_s$ (Å)	K_s (kcal/mol/Å^2)
H	4.52719	15.17433	1	0.371	2037.201
He	9.66	29.84	1	1.3	1619.411
Li	3.006	4.772	1	1.557	13.64832
Be	4.877	8.886	1	1.24	59.29709
B	5.11	9.5	1	0.822	109.592
C	5.41477	10.25602	1	0.759	198.8405
N	6.87577	10.26467	1	0.715	301.8761
O	9.7139	14.66128	1	0.669	414.0445
F	9.71494	17.7886	1	0.706	596.1646
Ne	11.04	21.1	1	1.768	842.1173
Na	2.843	4.592	1	2.085	13.77286
Mg	3.951	7.386	1	1.5	31.32676
Al	4.06	7.18	1	1.201	48.8329

Si	4.80466	6.71377	1	1.176	60.04769
P	6.02536	7.86352	1	1.102	91.4776
S	7.01035	8.95326	1	1.047	114.5047
Cl	7.81003	10.23353	1	0.994	152.3228
Ar	9.465	12.71	1	2.108	202.3422
K	2.421	3.84	1	2.586	7.71165
Ca	3.231	5.76	1	2	14.5642
Sc	3.395	6.16	1	1.75	18.65526
Ti	3.47	6.76	1	1.607	22.74409
V	3.65	6.82	1	1.47	26.77933
Cr	3.415	7.73	1	1.402	28.62618
Mn	3.325	8.21	1	1.533	35.32593
Fe	3.76	8.28	1	1.393	39.53139
Co	4.105	8.35	1	1.406	44.27516
Ni	4.465	8.41	1	1.398	48.8329
Cu	3.729	5.002	1	1.434	53.55866

Zn	5.106	8.57	1	1.4	57.75021
Ga	3.641	6.32	1	1.211	40.89454
Ge	4.80386	6.71243	1	1.189	56.86022
As	5.41473	7.5831	1	1.204	77.04494
Se	6.05692	8.40969	1	1.224	88.08056
Br	7.79	8.79002	1	1.141	108.8733
Kr	8.505	11.43	1	2.27	133.6595
Rb	2.331	3.692	1	2.77	7.02929
Sr	3.024	4.88	1	2.415	12.03129
Y	3.83	5.62	1	1.998	14.62836
Zr	3.4	7.1	1	1.758	18.55104
Nb	3.55	6.76	1	1.603	21.15055
Mo	3.465	7.51	1	1.53	25.94248
Tc	3.29	7.98	1	1.5	29.12839
Ru	3.575	8.03	1	1.5	34.58997
Rh	3.975	8.01	1	1.509	38.61206

Pd	4.32	8	1	1.544	69.17994
Ag	4.436	6.268	1	1.622	48.97695
Cd	5.034	7.914	1	1.6	45.11735
In	3.506	5.792	1	1.404	32.55526
Sn	4.62392	6.45025	1	1.354	52.87639
Sb	4.56949	6.45124	1	1.404	50.31268
Te	6.02877	6.80311	1	1.38	60.37522
I	6.1548	7.50909	1	1.333	62.06798
Xe	7.595	9.95	1	2.459	82.11269
Cs	2.183	3.422	1	2.984	5.58842
Ba	2.814	4.792	1	2.442	8.36432
La	2.8355	5.483	1	2.071	10.67729
Ce	2.774	5.384	1	1.925	11.21837
Pr	2.858	5.128	1	2.007	11.77531
Nd	2.8685	5.241	1	2.007	10.57528
Pm	2.881	5.346	1	2	11.03202

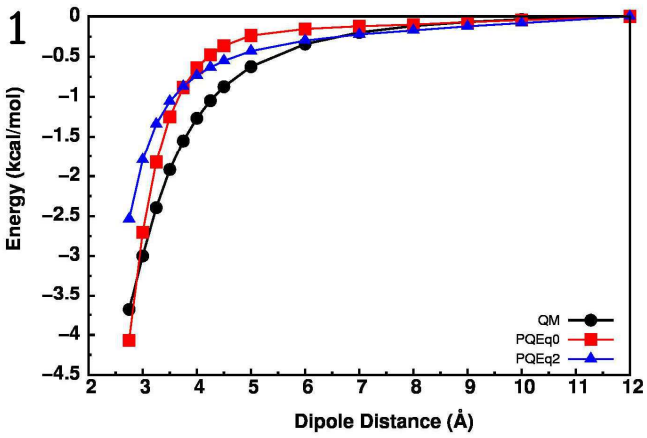
Sm	2.9115	5.439	1	1.978	11.52999
Eu	2.8785	5.575	1	2.227	11.98786
Gd	3.1665	5.949	1	1.968	14.13037
Tb	3.018	5.668	1	1.954	13.02211
Dy	3.0555	5.743	1	1.934	13.55362
Ho	3.127	5.782	1	1.925	14.0705
Er	3.1865	5.829	1	1.915	14.62836
Tm	3.2514	5.8658	1	2	15.23228
Yb	3.2889	5.93	1	2.158	15.88822
Lu	2.9629	4.9258	1	1.896	15.16273
Hf	3.7	6.8	1	1.759	20.49776
Ta	5.1	5.7	1	1.605	25.34837
W	4.63	6.62	1	1.538	29.91565
Re	3.96	7.84	1	1.6	34.23337
Os	5.14	7.26	1	1.7	39.06632
Ir	5	8	1	1.866	43.69259

Pt	4.79	8.86	1	1.557	51.08672
Au	4.894	5.172	1	1.618	57.25236
Hg	6.27	8.32	1	1.6	66.14815
Tl	3.2	5.8	1	1.53	43.69259
Pb	3.9	7.06	1	1.444	47.5736
Bi	4.53181	7.32783	1	1.514	44.87347
Po	4.42943	8.40996	1	1.48	48.8329
At	4.53674	8.99576	1	1.47	55.34395
Rn	5.37	10.74	1	2.2	62.65353
Fr	2	4	1	2.3	6.83259
Ra	2.843	4.868	1	2.2	8.67007
Ac	2.835	5.67	1	2.108	10.34466
Th	3.175	5.81	1	2.018	10.34466
Pa	2.985	5.81	1	1.8	13.07337
U	3.341	5.706	1	1.713	13.33589
Np	3.549	5.434	1	1.8	13.38967

Pu	3.243	5.638	1	1.84	13.55362
Am	2.9895	6.007	1	1.942	14.25166
Cm	2.8315	6.379	1	1.9	14.43755
Bk	3.1935	6.071	1	1.9	14.62836
Cf	3.197	6.202	1	1.9	16.19823
Es	3.333	6.178	1	1.9	16.85603
Fm	3.4	6.2	1	1.9	13.95226
Md	3.47	6.22	1	1.9	18.24526
No	3.475	6.35	1	1.9	20.24779
Lr	3.5	6.4	1	1.9	0

2. Electrostatic Interaction Energy Curves

Figure S1: A comparison between QM (LACVP**++[1] or ERMLER**++[2] and B3LYP[3]) with PQEq and PQEq2 via the electrostatic interaction dipole energies. A subfigure is depicted for each plot to describe the direction of the dipole scan.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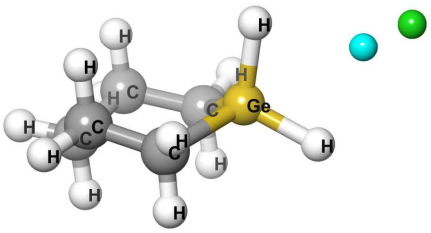
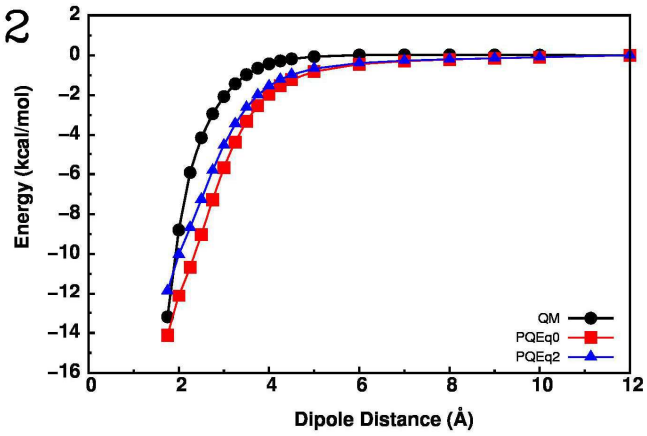
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2


H
C
Ge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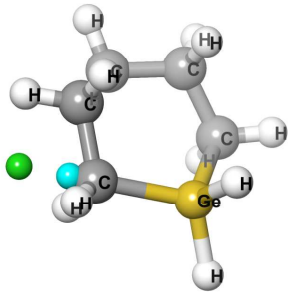
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2


H
C
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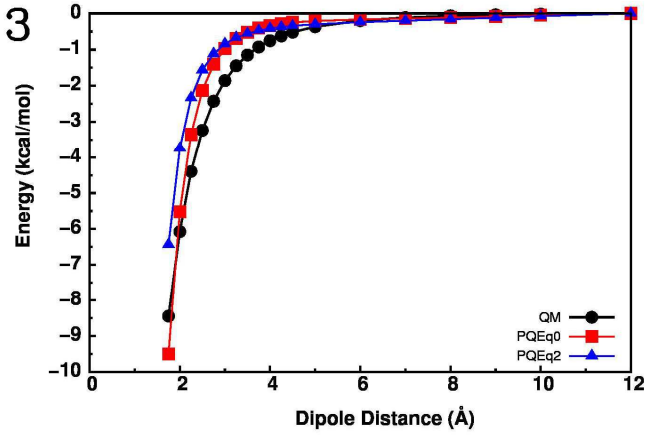
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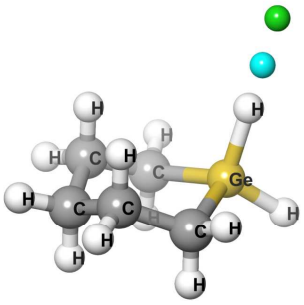
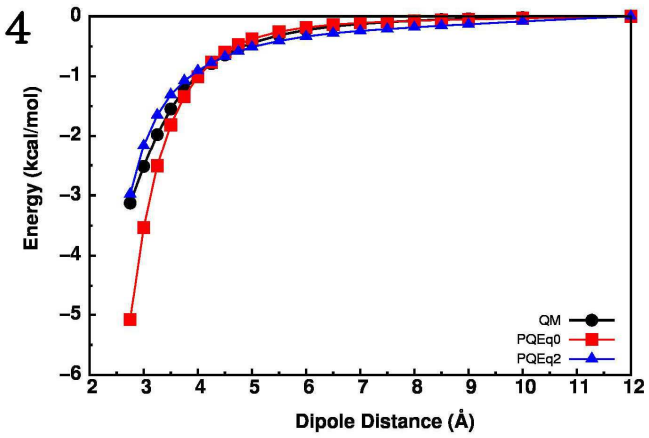
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2


H
C
Ge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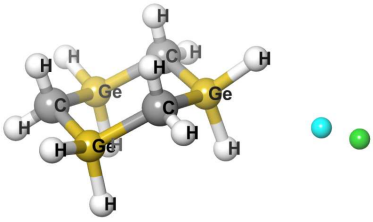
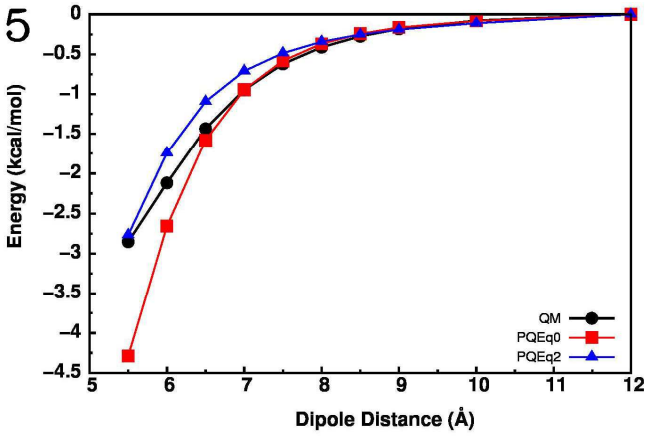
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

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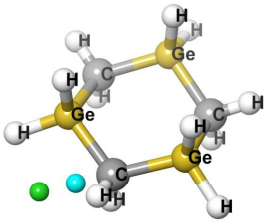
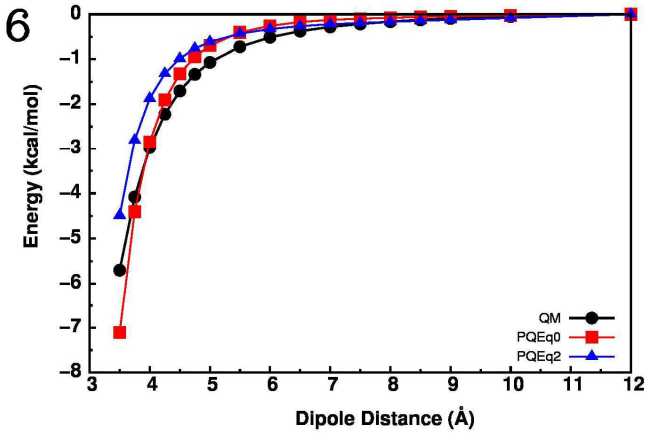
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

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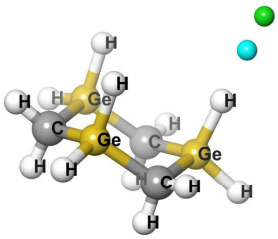
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2



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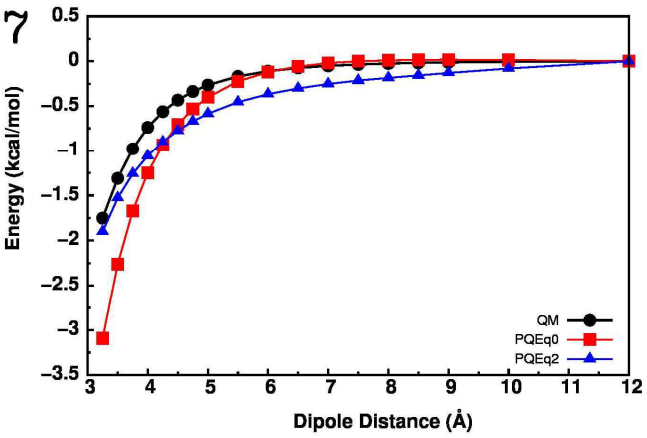
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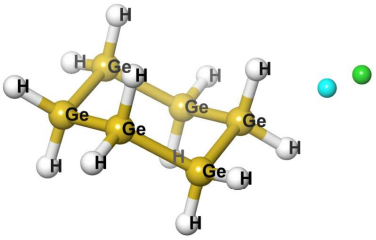
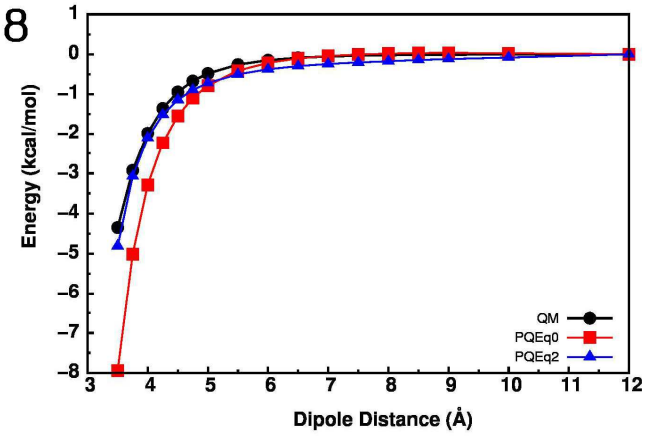
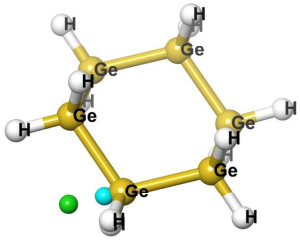
Dipole Distance (Å)
QM
PQEq0
PQEq2

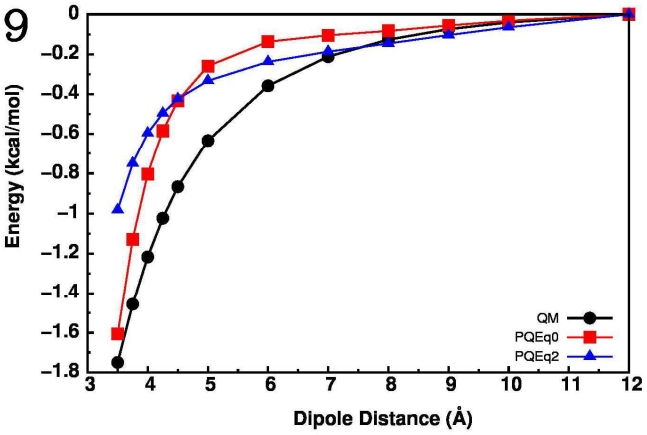

H
Ge

8


Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2


H
Ge

9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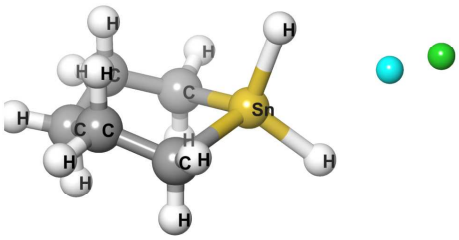
Dipole Distance (Å)
QM
PQEq0
PQEq2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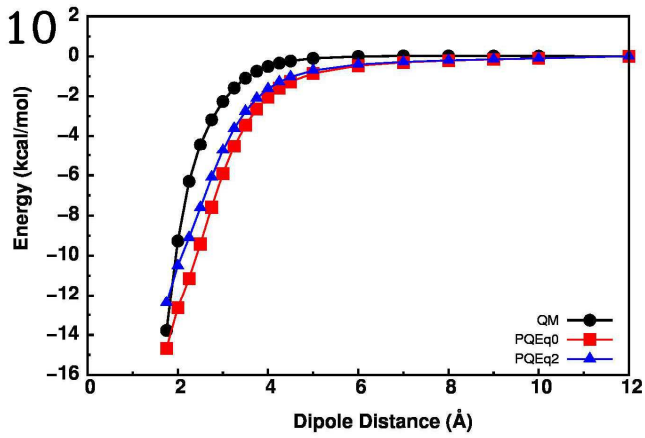
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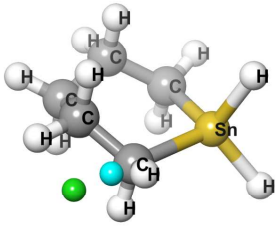
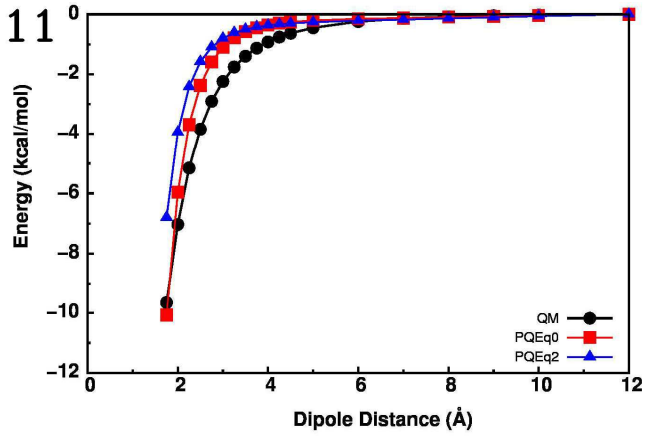
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

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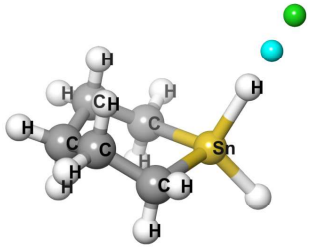
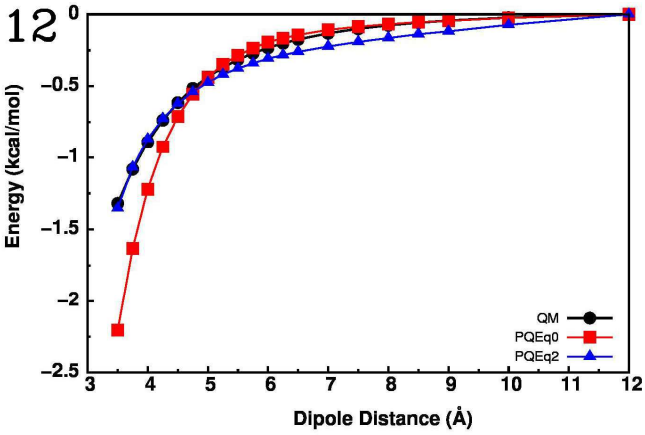
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

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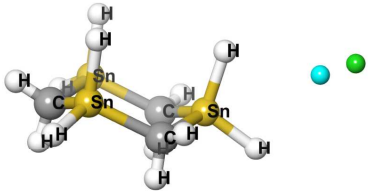
Dipole Distance (Å)
QM
PQEq0
PQEq2



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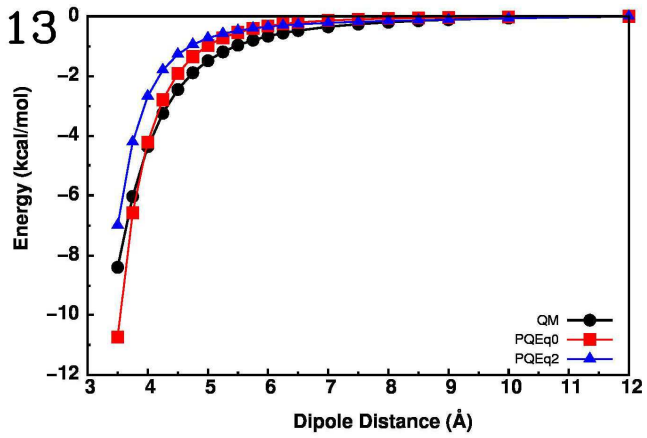
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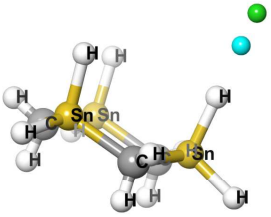
Dipole Distance (Å)
QM
PQEq0
PQEq2



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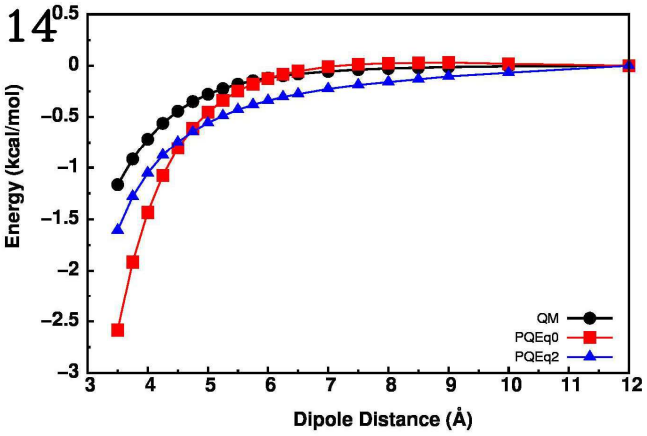
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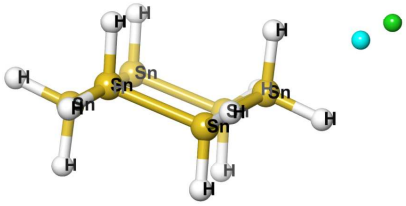
Dipole Distance (Å)
QM
PQEq0
PQEq2



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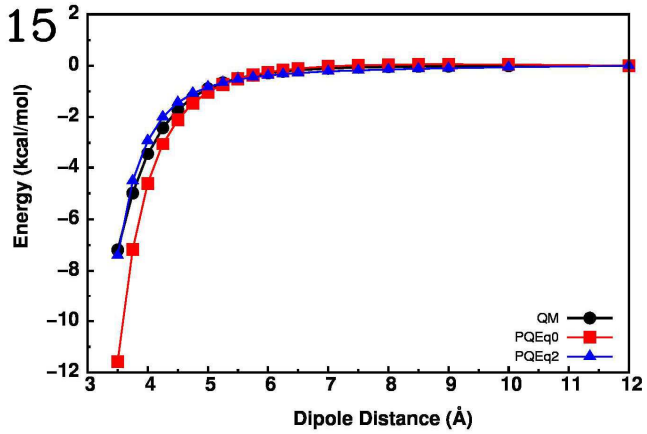
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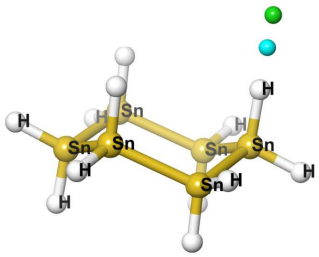
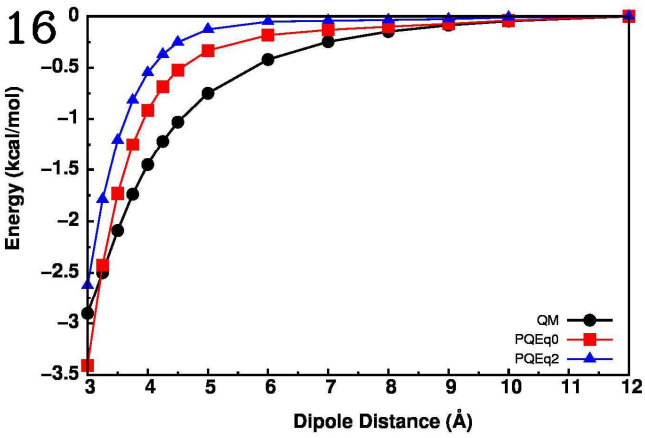
Dipole Distance (Å)
QM
PQEq0
PQEq2

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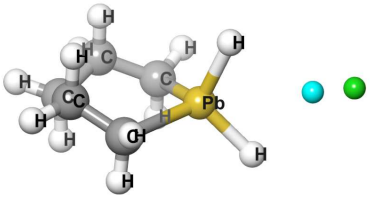
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2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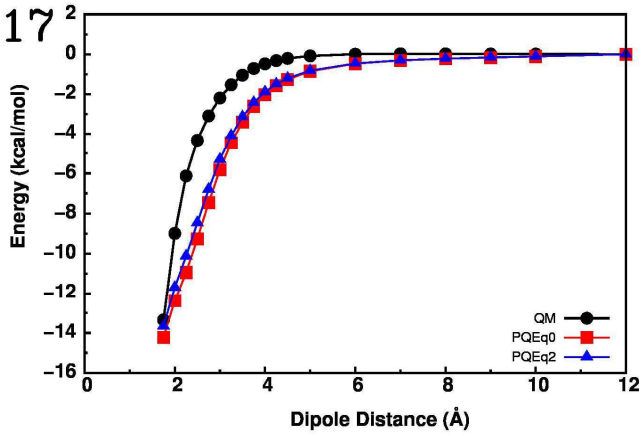
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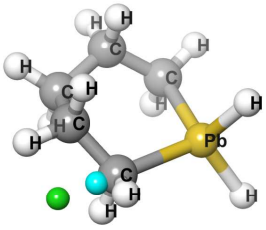
Dipole Distance (Å)
QM
PQEq0
PQEq2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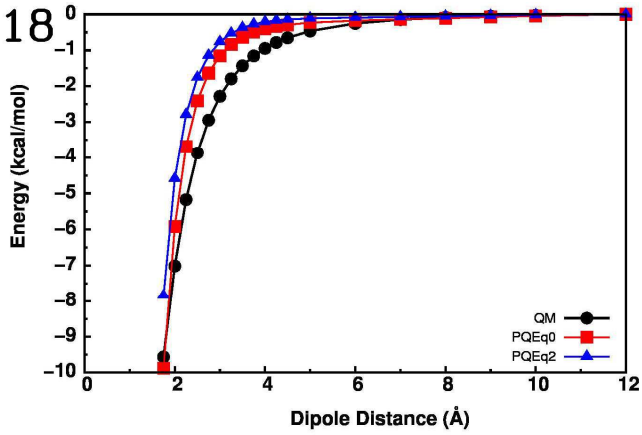
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Dipole Distance (Å)
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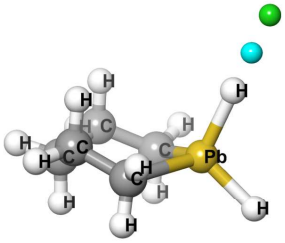
PQEq2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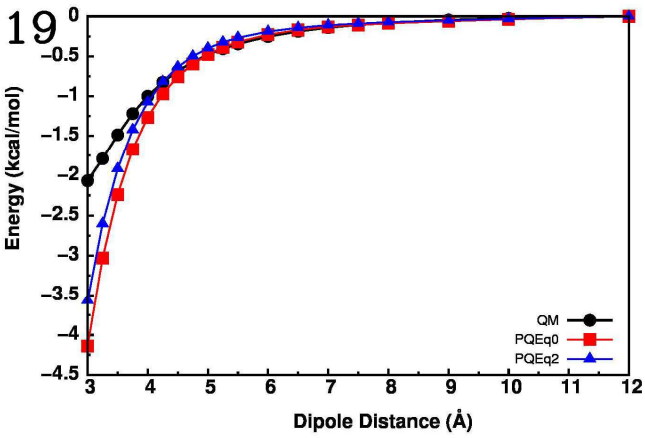
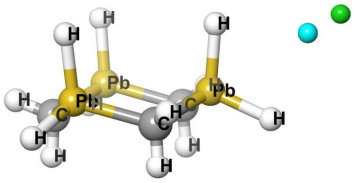
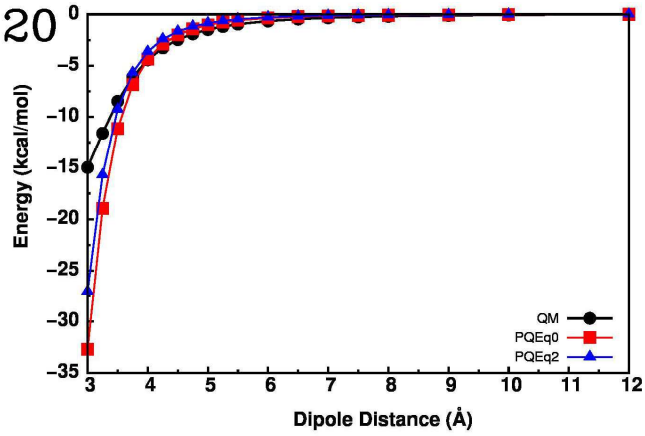
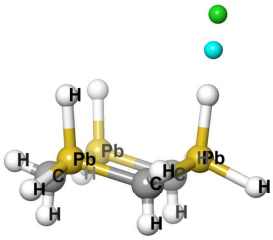
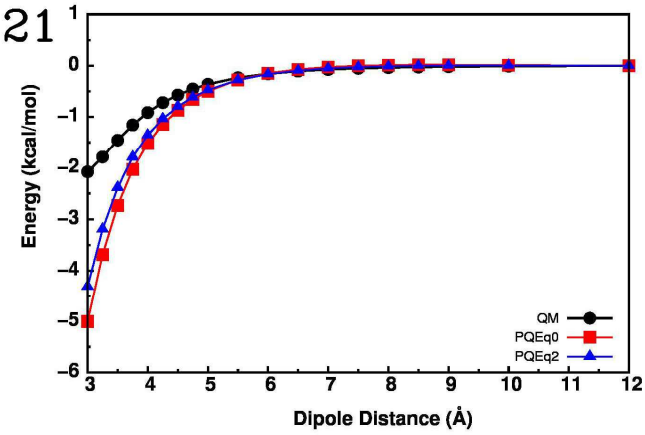
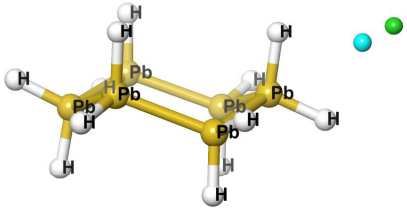

19
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

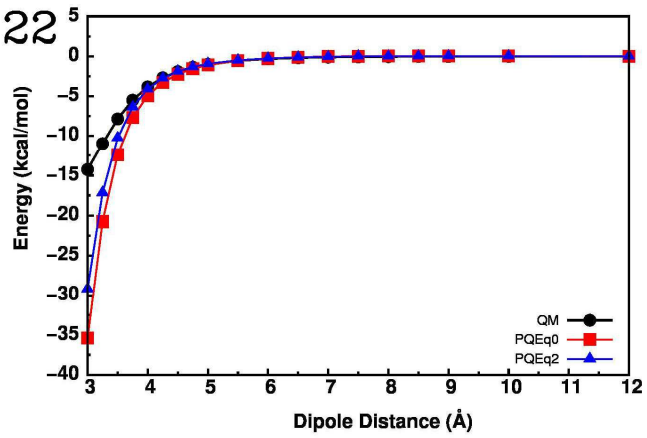


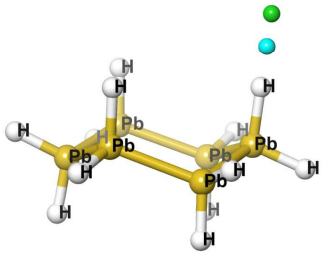

20
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

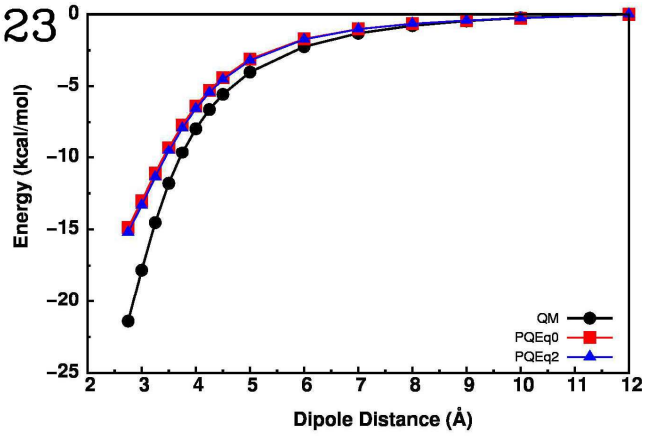


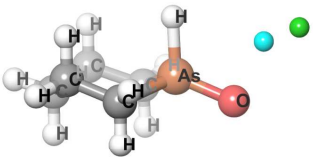

21
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

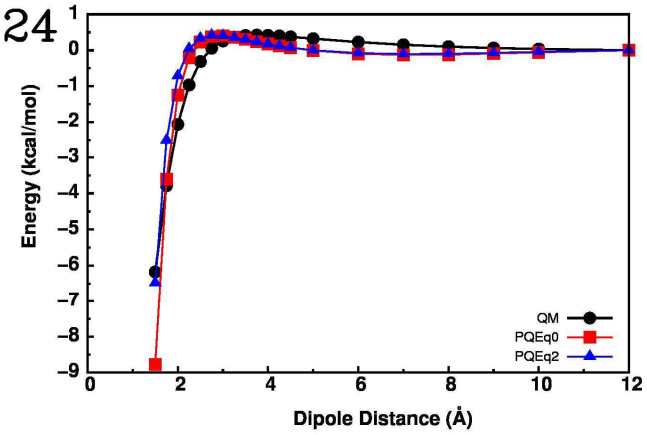


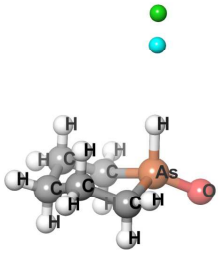

22
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

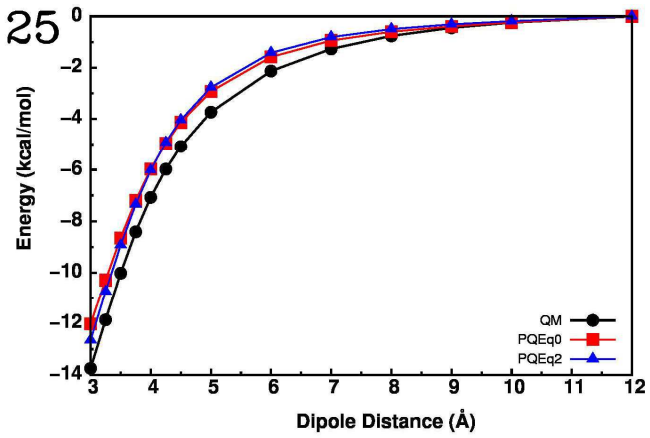

Pb
H

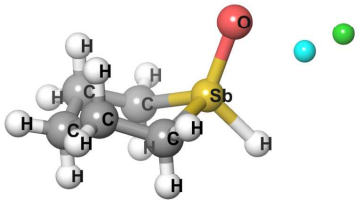

23
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

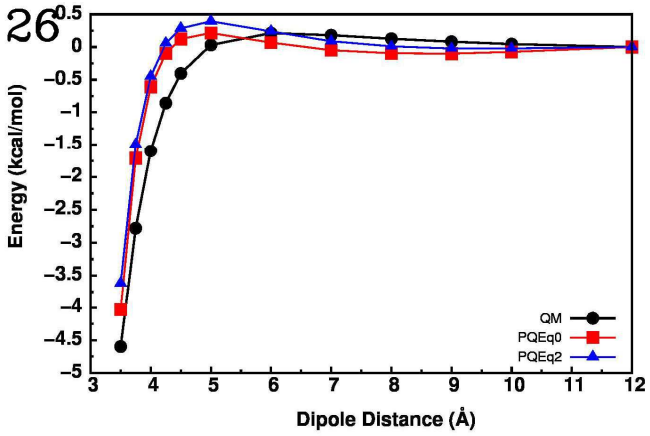

As
O
C
H

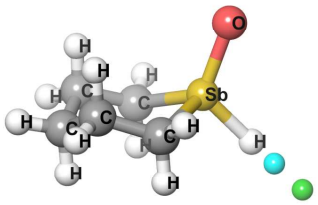

24
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

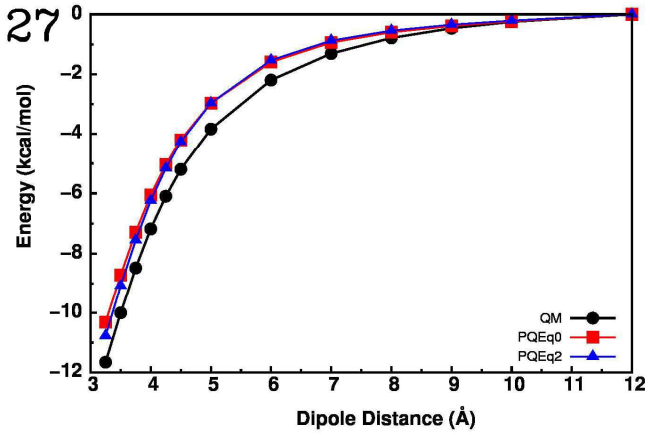

As
O
C
H

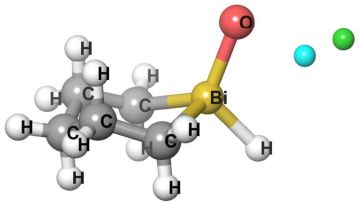

25
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

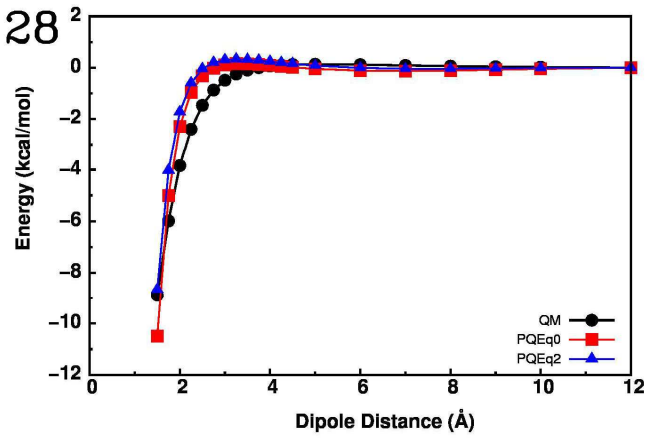

O
Sb

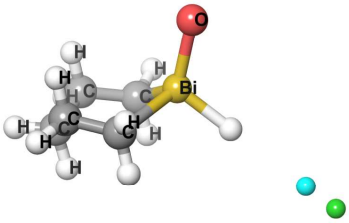

26
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

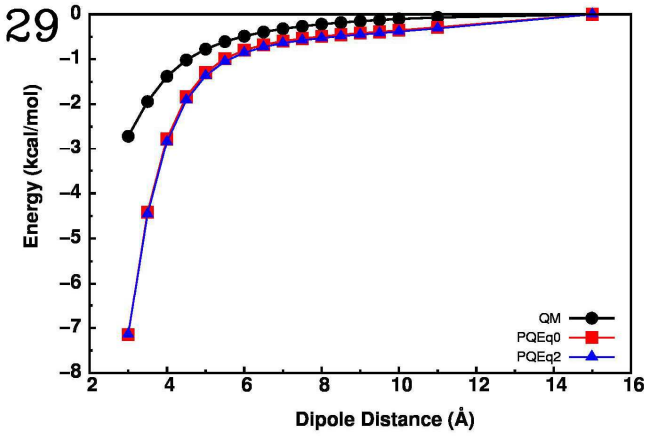

O
Sb

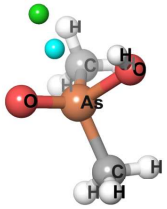

27
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

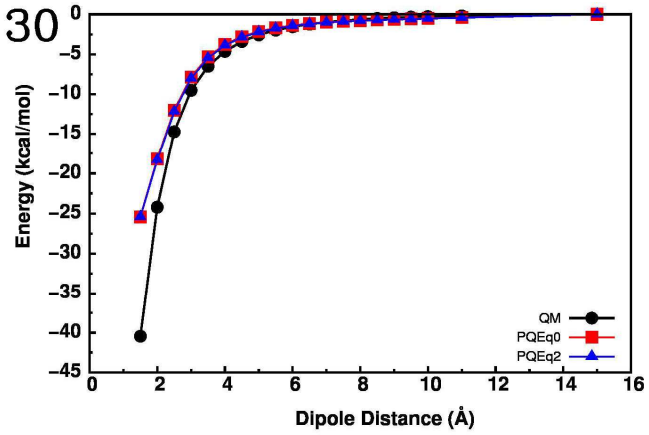

O
Bi

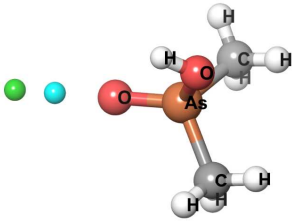

28
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

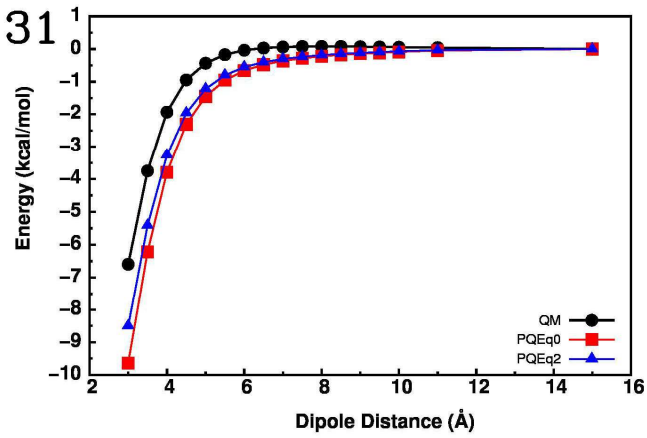

O
H
C
Bi

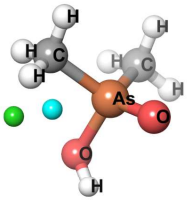

29
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

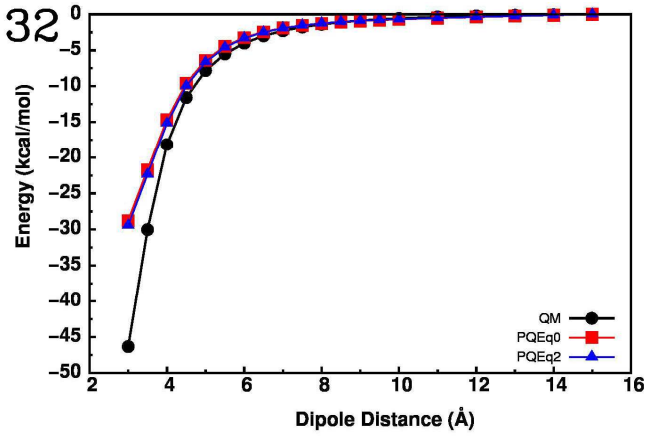

H
C
O
As

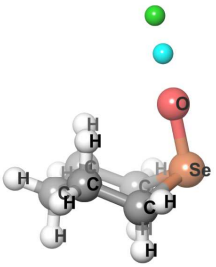

30
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

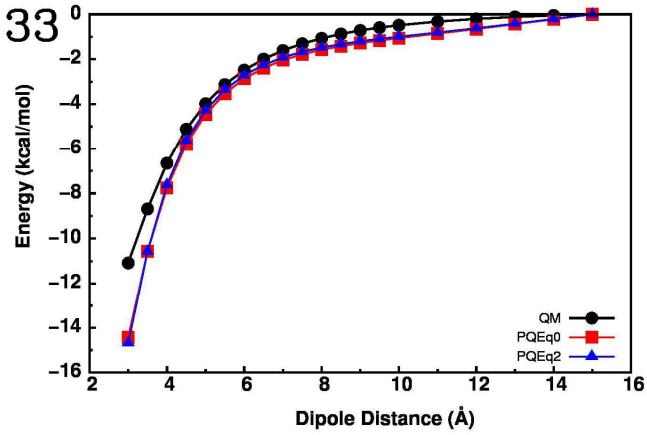

H
C
O
As

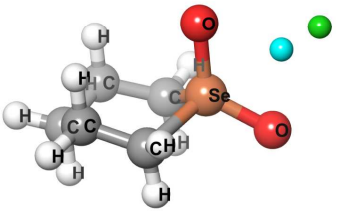

31
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

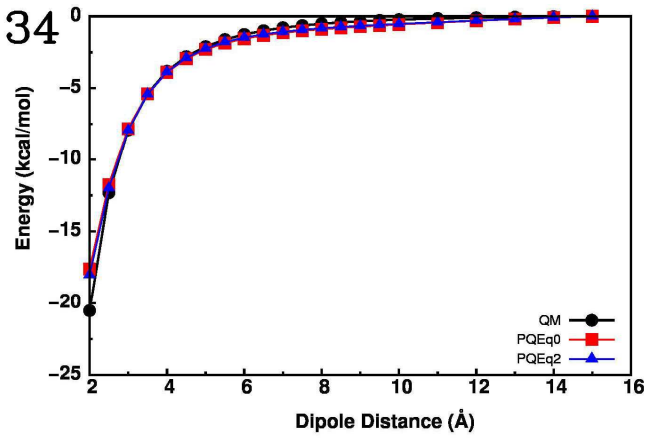

As
O
H
C

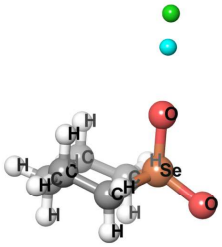

32
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

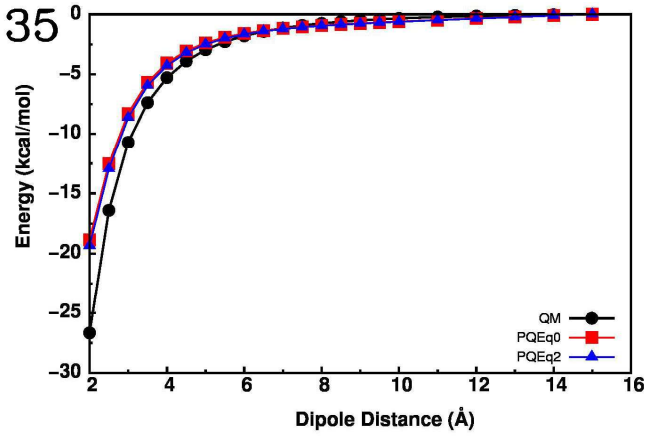

O
Se
H
C

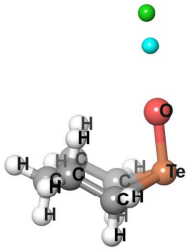

33
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

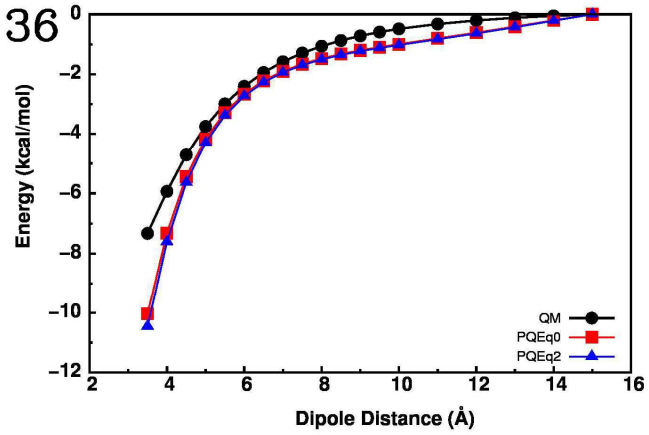

O
Se
H
C

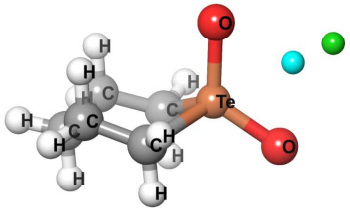

34
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

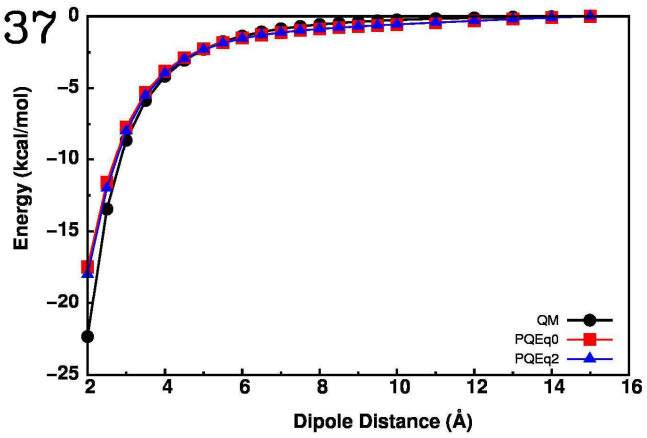

O
H
C
Se

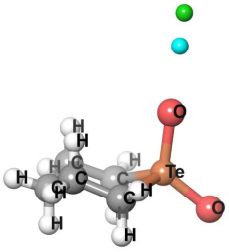

35
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

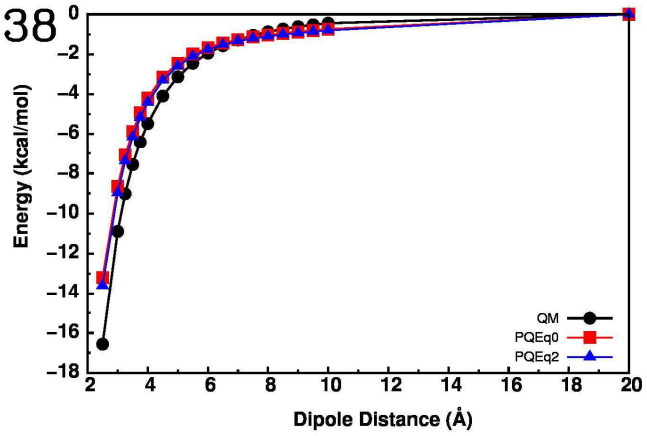

O
H
C
Te

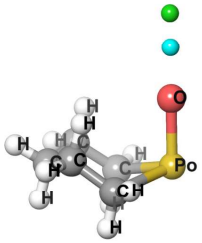

36
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

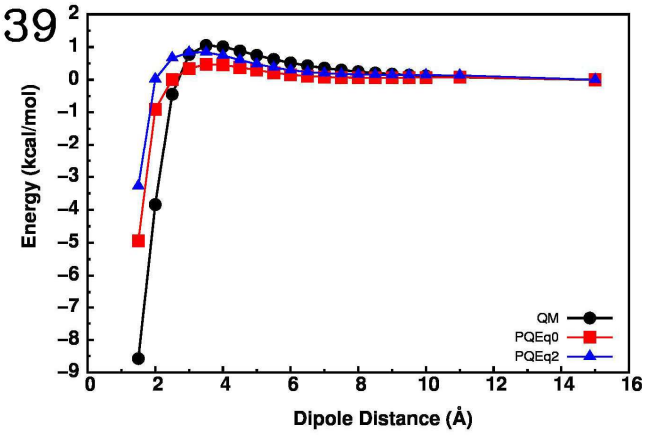

O
H
C
Te

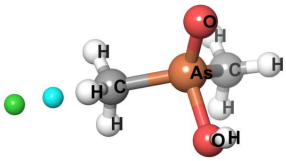

37
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

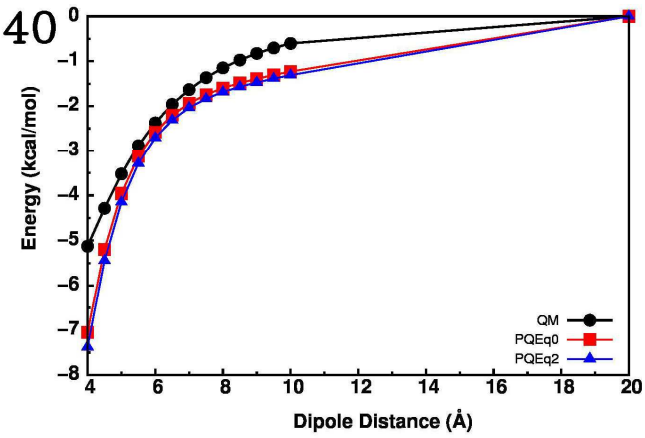

O
H
C
Te

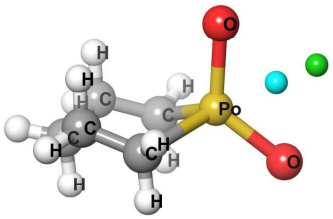

38
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

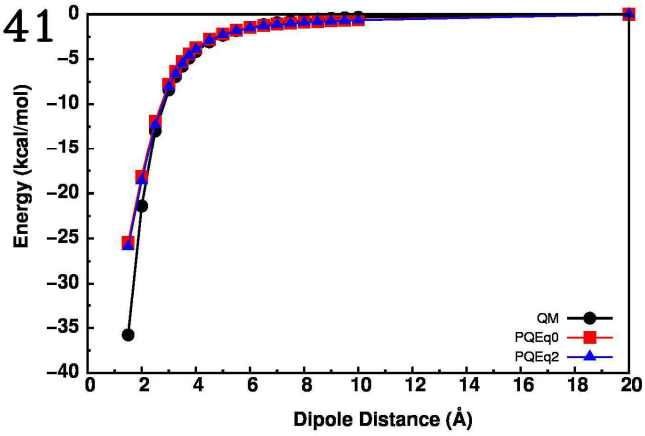

O
H
C
Po

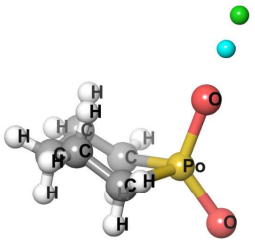

39
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

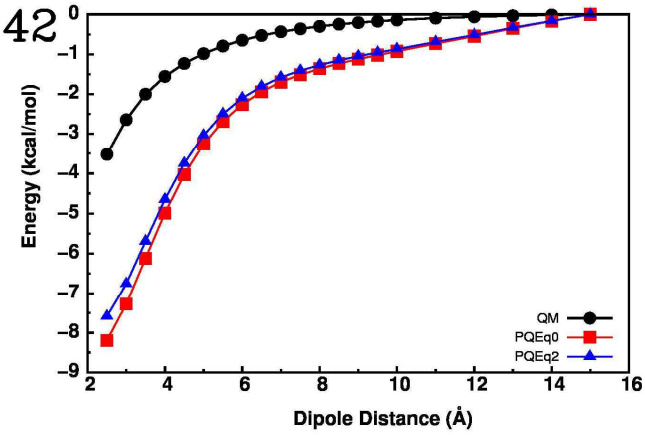

O
H
C
As
OH

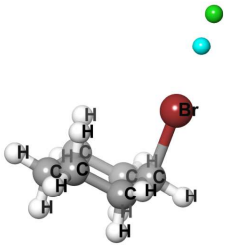

40
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

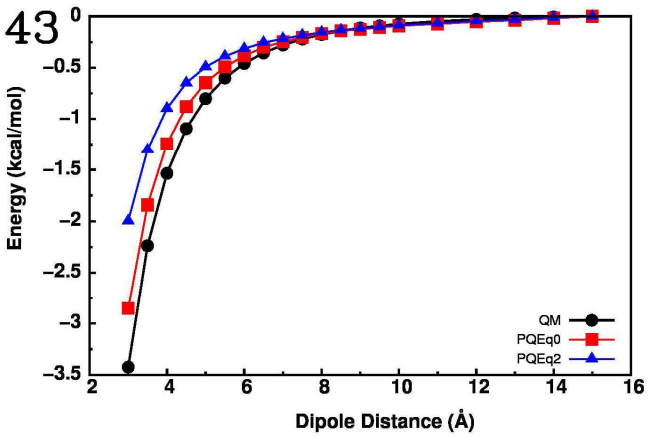

O
H
C
Po
O

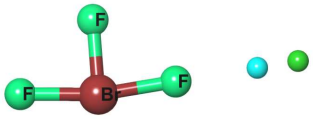

41
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

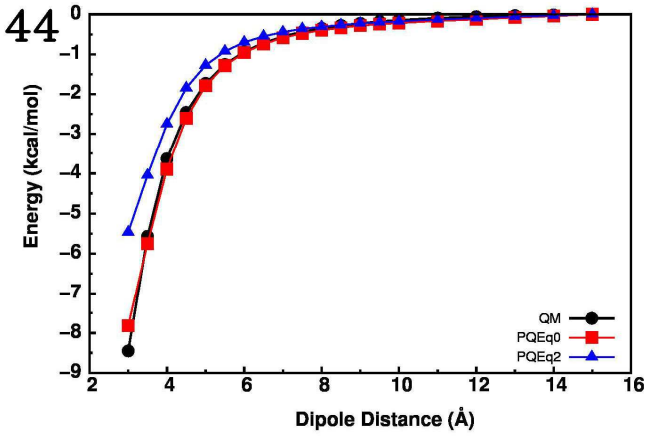

O
H
C
Po
O

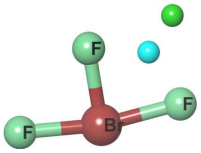

42
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

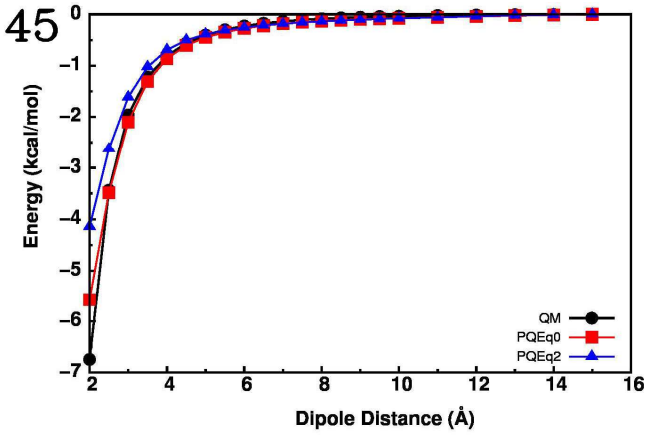

Br
H
C

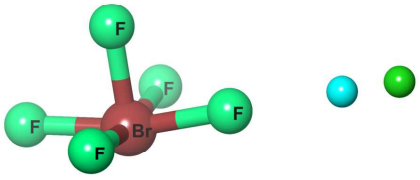

43
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2


F
F
B
F


44
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2


F
F
B
F


45
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2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F
F
Br
F
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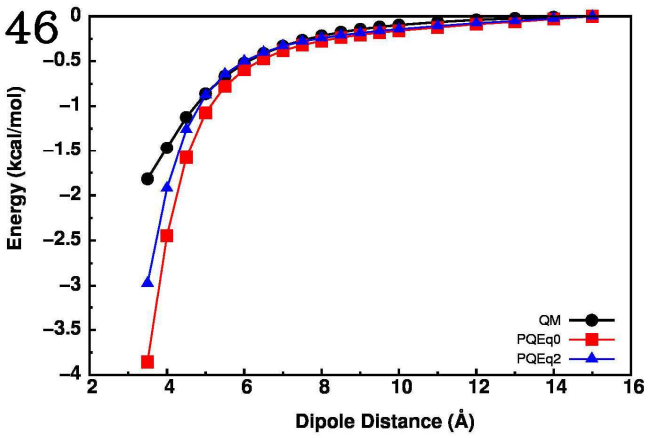
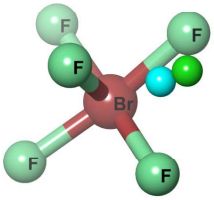

46
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2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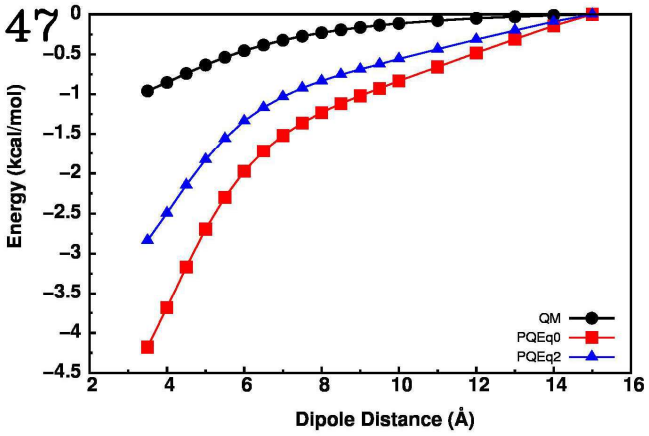
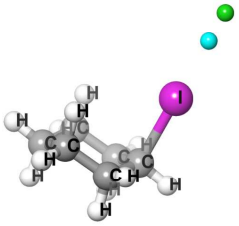
F
F
Br
F
F


47
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2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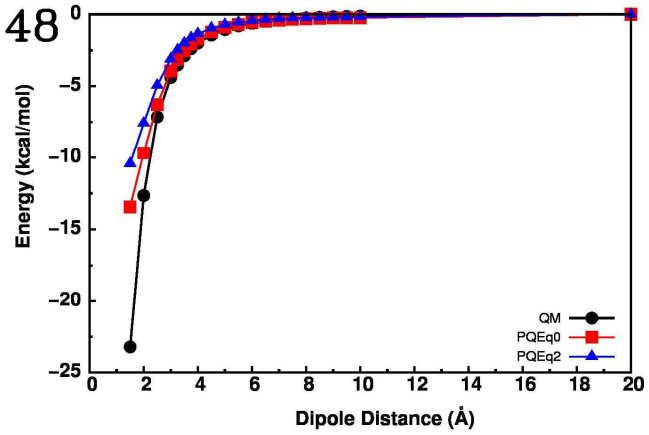
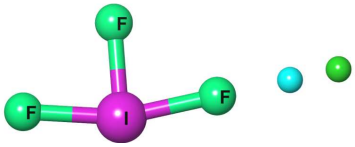

48
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2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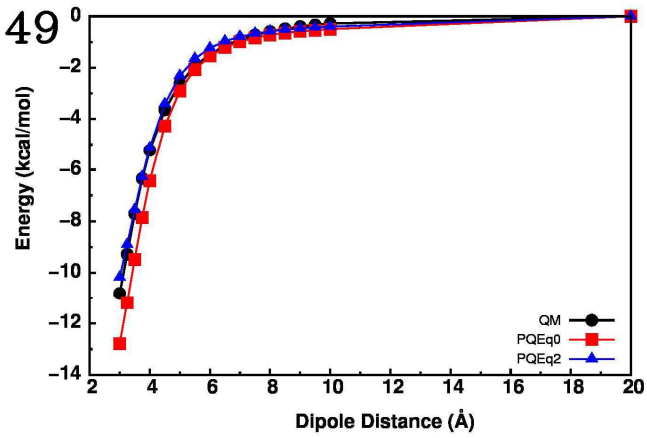
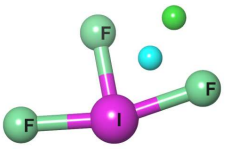

49
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2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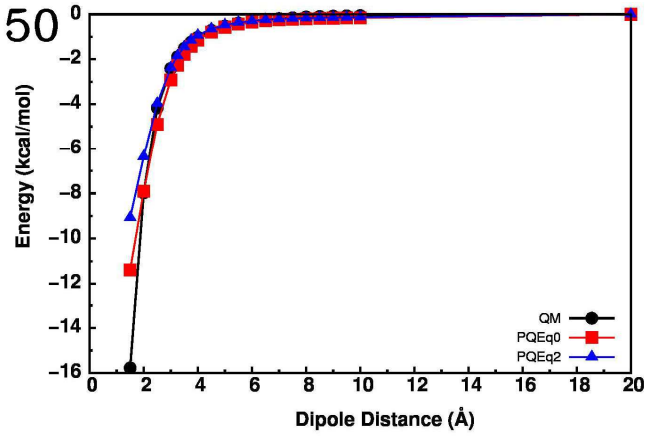
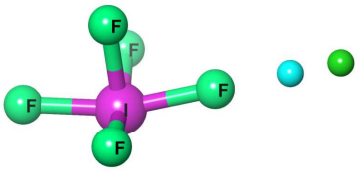

50
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2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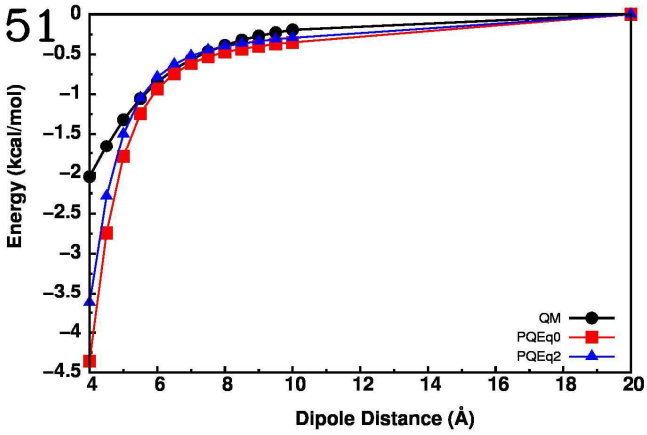
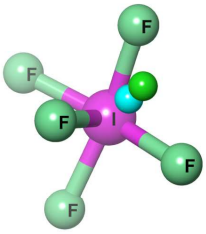
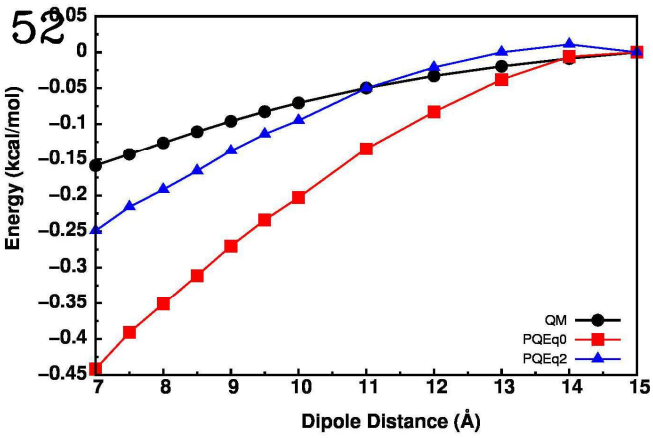
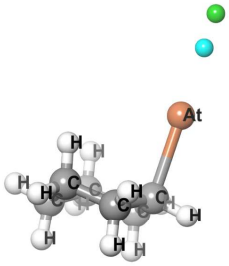
F
F
F
I


51
Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

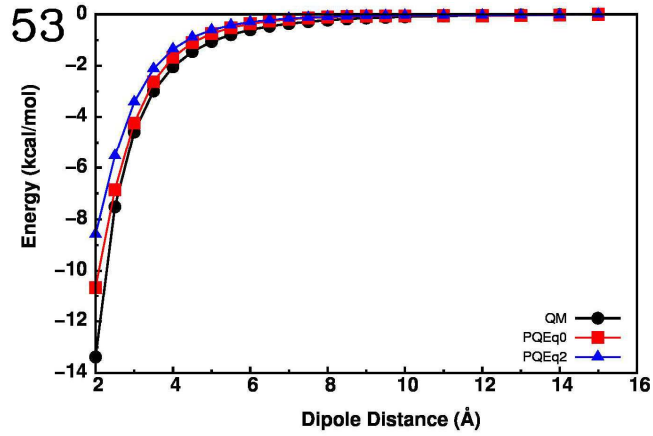

F
F
F
I
F
F

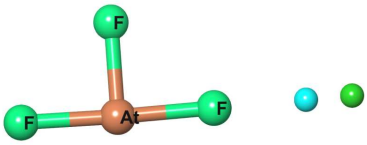
52


Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

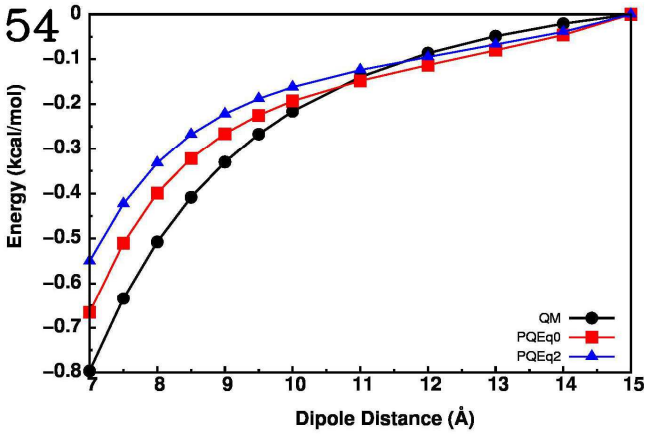

At
H
C

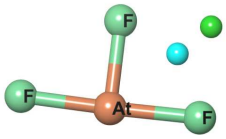
53

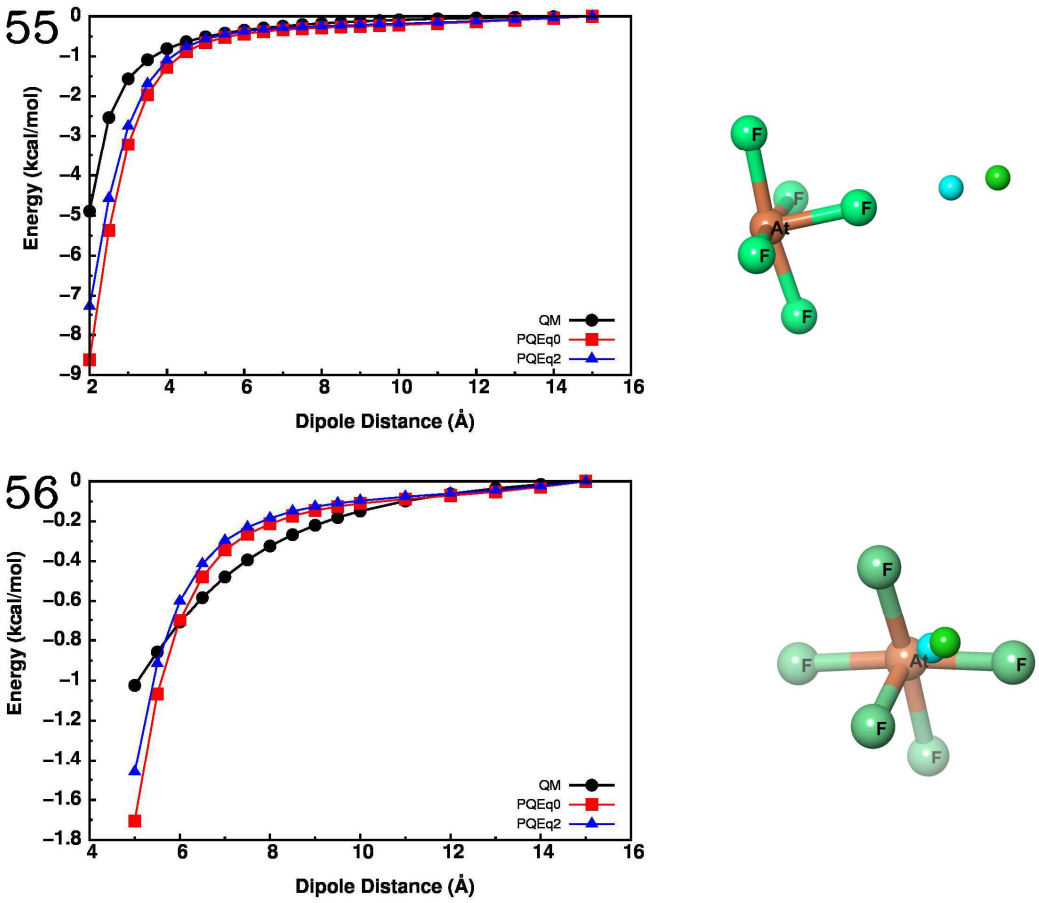

Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2


F
At

54

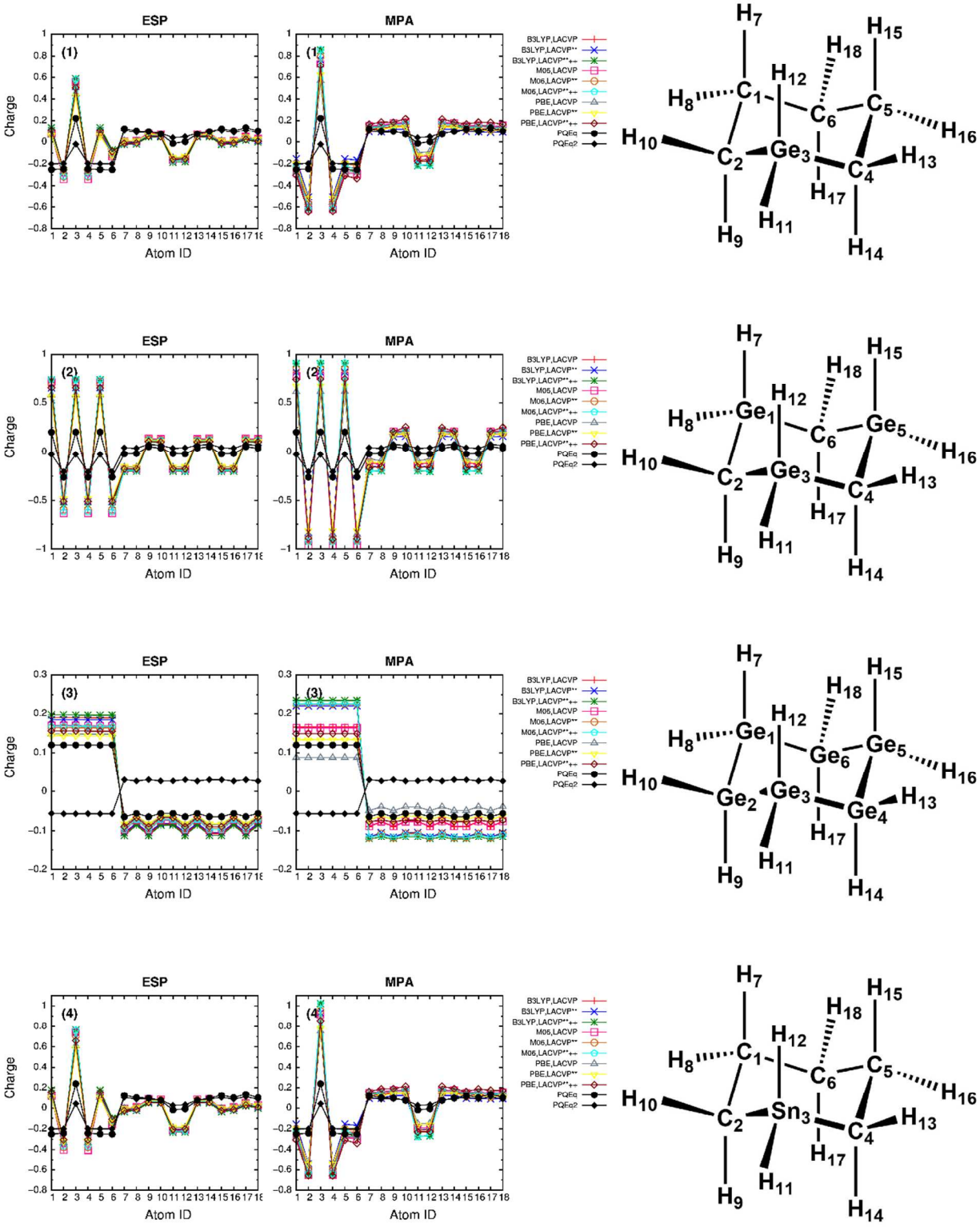

Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq0
PQEq2

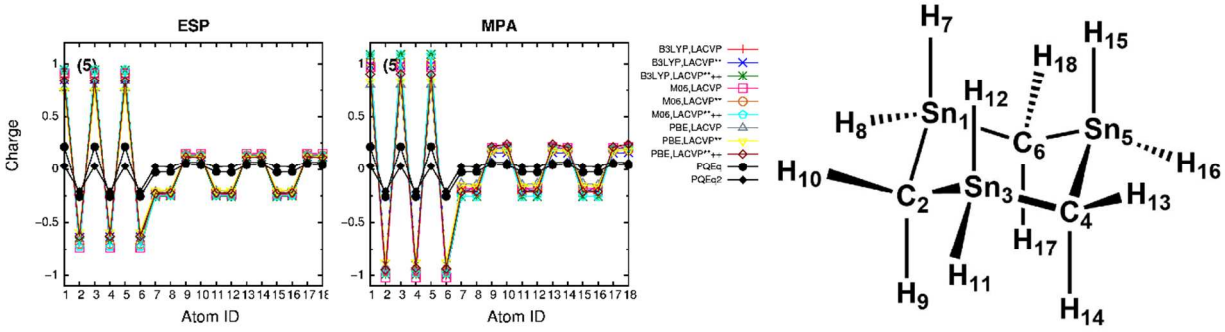

F
At

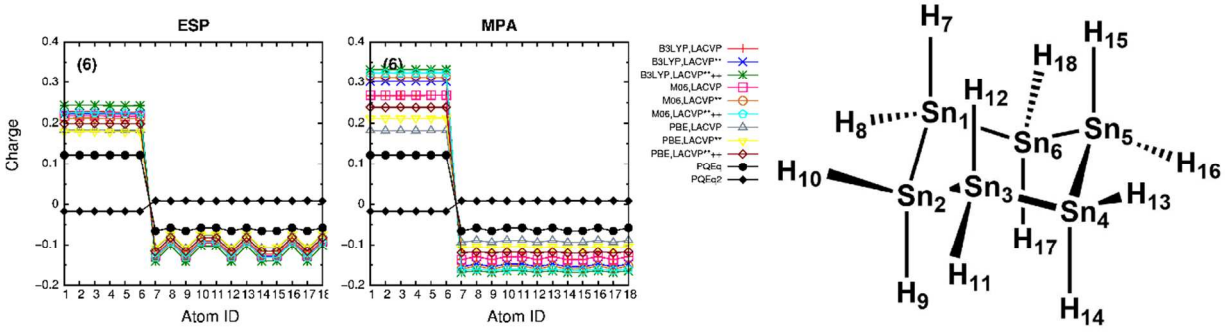


3. Charge Comparison between PQEq, PQEq2, and QM

Figure S2: A comparison of the partial charge calculations using electrostatic potentials (ESP) and Mulliken population analysis (MPA) with PQEq, PQEq2, and combinations of B3LYP, M06, PBE with LACVP, LACVP++, and LACVP++** (or the corresponding ERMLER2 equivalent for Po and At).


ESP
MPA
(1)
(2)
(3)
(4)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H15
H18
H12
H8
C1
C6
C5
H16
H10
C2
Ge3
C4
H13
H17
H11
H9
H14
Ge1
Ge5
Ge6
Ge2
Ge4
Sn3


ESP
MPA
(5)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H15
H18
H12
H8
Sn1
C6
Sn5
H16
H10
C2
Sn3
C4
H13
H17
H11
H9
H14


ESP
MPA
(6)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H15
H18
H12
H8
Sn1
Sn6
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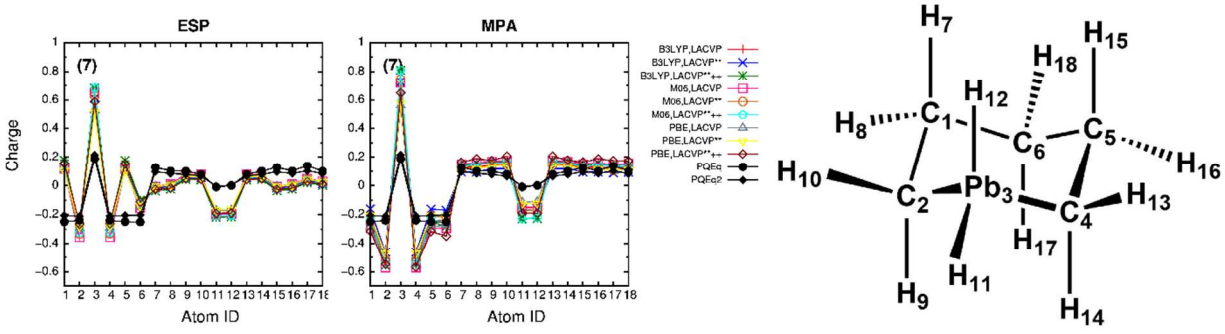
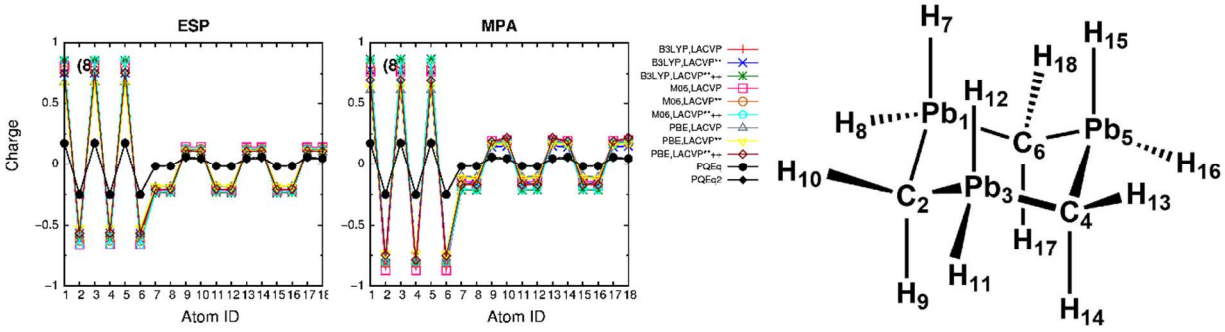
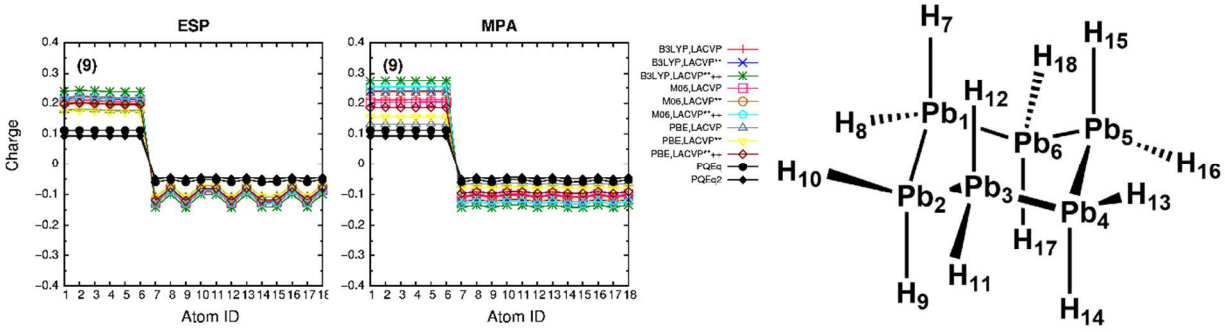
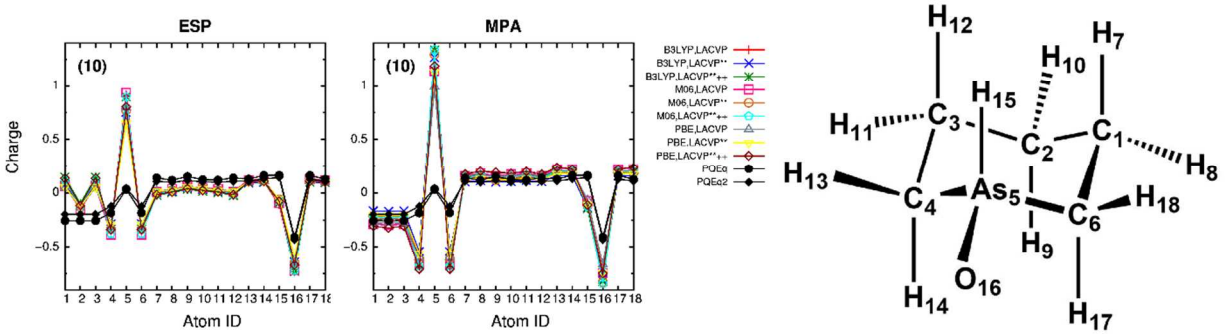
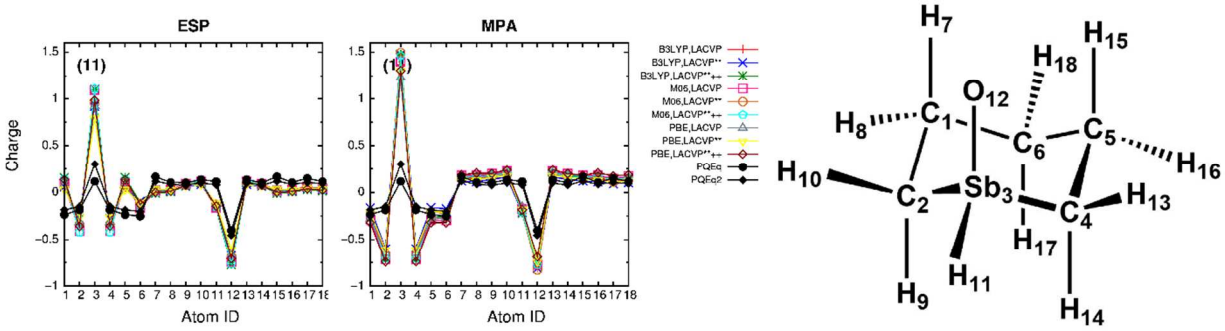
H10
Sn2
Sn3
Sn4
H13
H17
H11
H9
H14


ESP
MPA
(7)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H15
H18
H12
H8
C1
C6
C5
H16
H10
C2
Pb3
C4
H13
H17
H11
H9
H14


ESP
MPA
(8)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H15
H18
H12
H8
Pb1
C6
Pb5
H16
H10
C2
Pb3
C4
H13
H17
H11
H9
H14


ESP
MPA
(9)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H15
H18
H12
H8
Pb1
Pb6
Pb5
H16
H10
Pb2
Pb3
H13
Pb4
H17
H11
H9
H14


ESP
MPA
(10)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H12
H7
H10
H15
H11
C3
C2
C1
H8
H13
C4
As5
C6
H18
H9
O16
H14
H17


ESP
MPA
(11)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H15
H18
O12
H8
C1
C6
C5
H16
H10
C2
Sb3
C4
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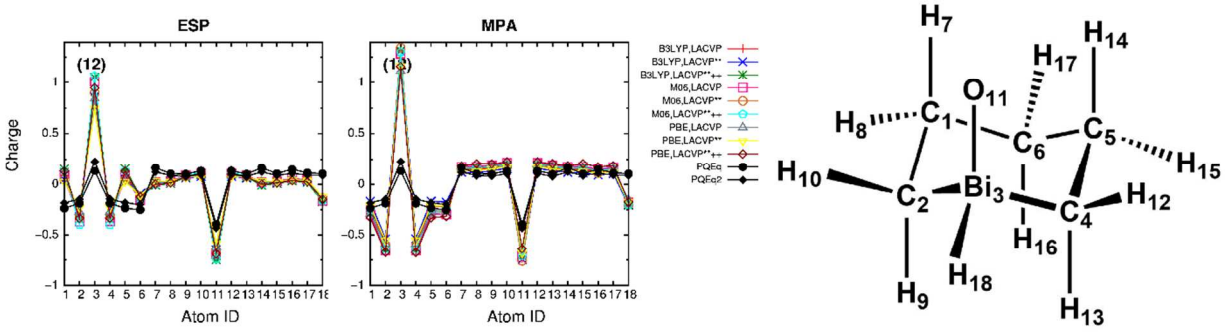
H17
H11
H9
H14


ESP
MPA
(12)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H14
H17
O11
H8
C1
C6
C5
H15
H10
C2
Bi3
C4
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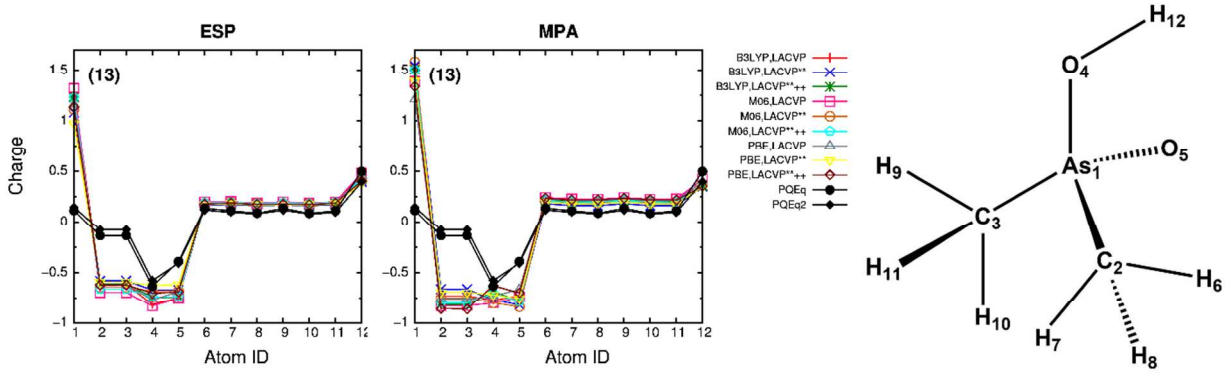
H16
H18
H9
H13


ESP
MPA
(13)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M06,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H12
O4
O5
As1
H9
C3
C2
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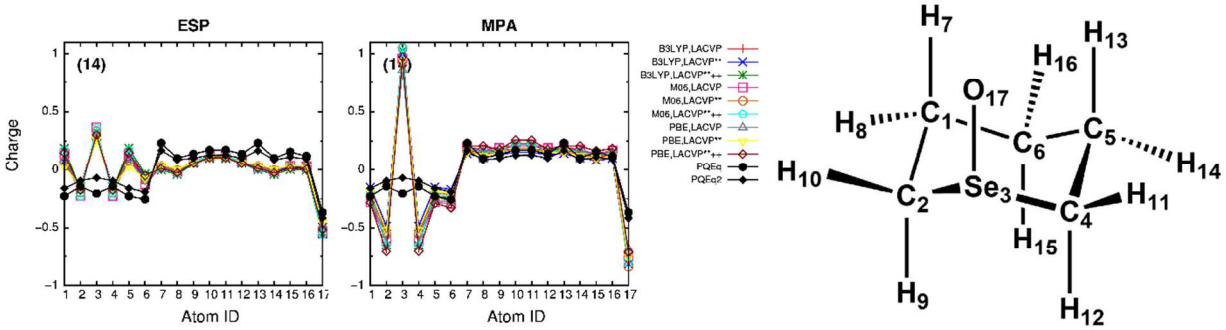
H11
H10
H7
H8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MPA
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Charge
Atom ID
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B3LYP,LACVP**
B3LYP,LACVP**++
M06,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H13
H16
O17
H8
C1
C6
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Se3
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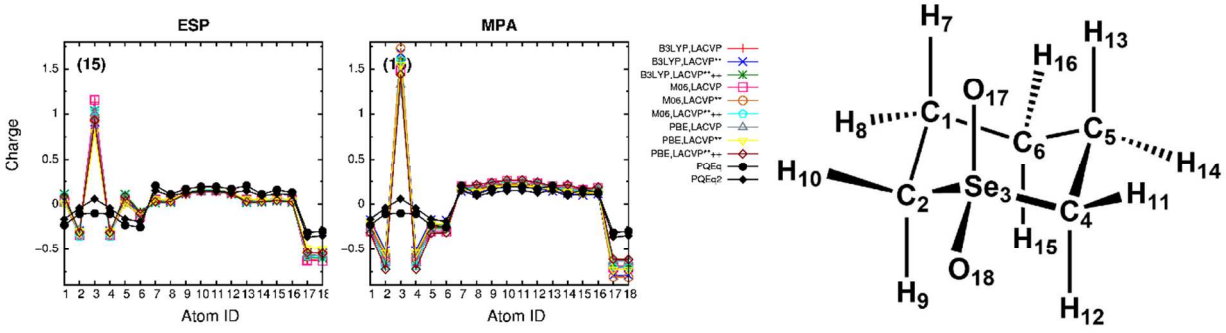
H11
H15
H9
H12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MPA
(15)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M06,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H13
H16
O17
H8
C1
C6
C5
H14
H10
C2
Se3
C4
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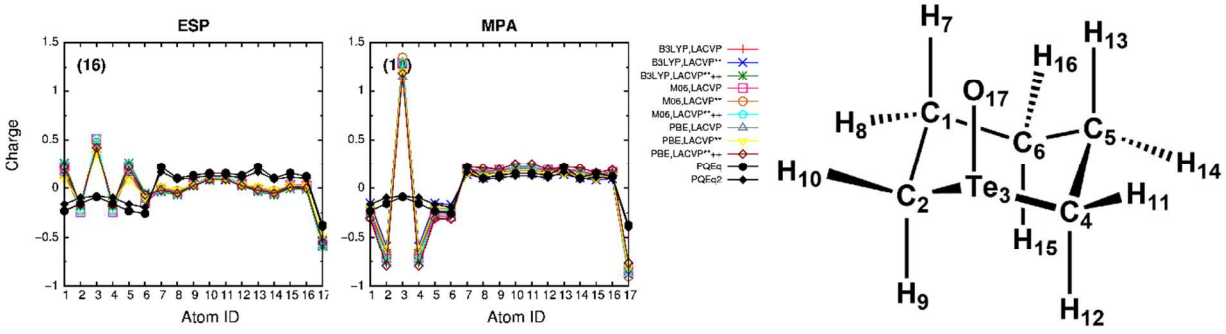
H15
O18
H9
H12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M06,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H13
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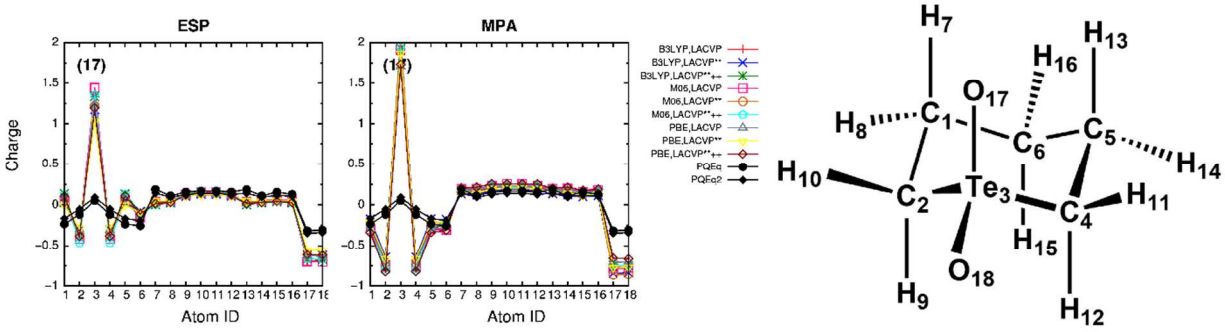
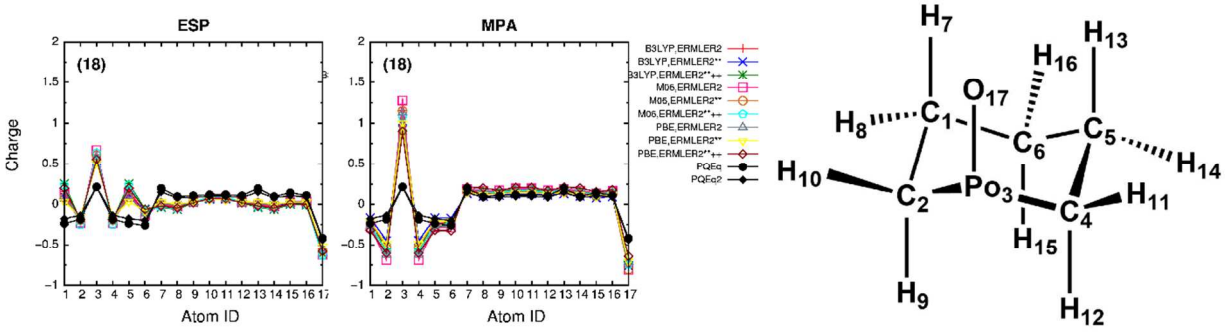
H11
H15
H9
H12


ESP
MPA
(17)
(17)
Charge
Atom ID
B3LYP,LACVP
B3LYP,LACVP**
B3LYP,LACVP**++
M05,LACVP
M06,LACVP**
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H13
H16
O17
H8
C1
C6
C5
H14
H10
C2
Te3
C4
H11
H15
O18
H9
H12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M06,ERMLER2**++
PBE,ERMLER2
PBE,ERMLER2**
PBE,ERMLER2**++
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PQEq2
H7
H13
H16
O17
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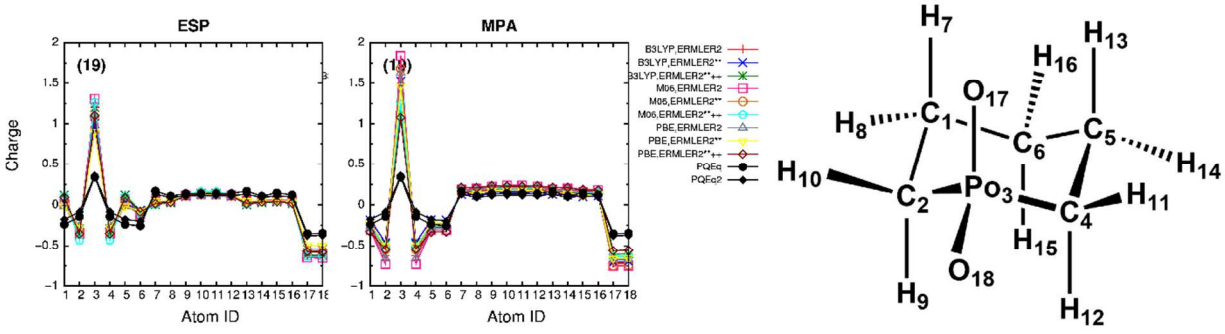
C1
C6
C5
H14
H10
C2
Po3
C4
H11
H15
H9
H12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M06,ERMLER2**
M06,ERMLER2**++
PBE,ERMLER2
PBE,ERMLER2**
PBE,ERMLER2**++
PQEq
PQEq2
H7
H13
H16
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C5
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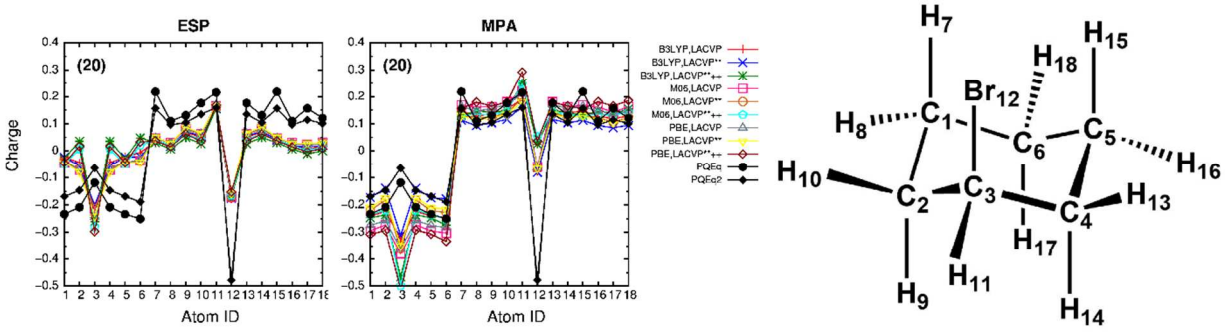
H10
C2
Po3
C4
H11
H15
O18
H9
H12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M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2
H7
H15
H18
Br12
H8
C1
C6
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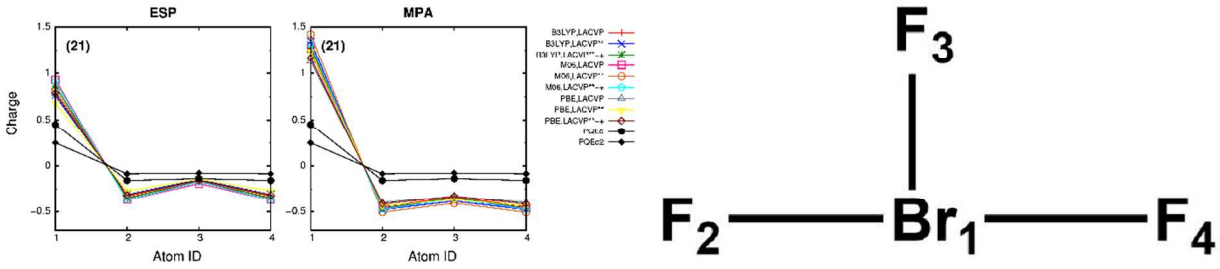
H17
H11
H9
H14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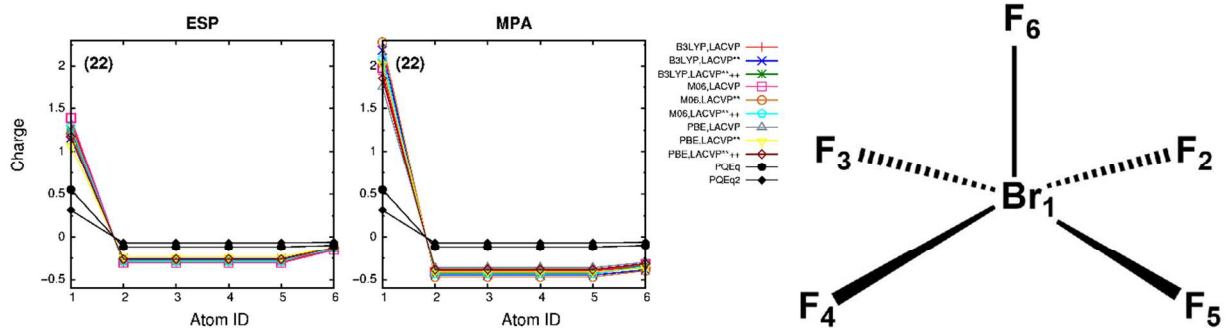
PBE,LACVP**
PQEq
PQEq2
F3
F2
Br1
F4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PQEq2
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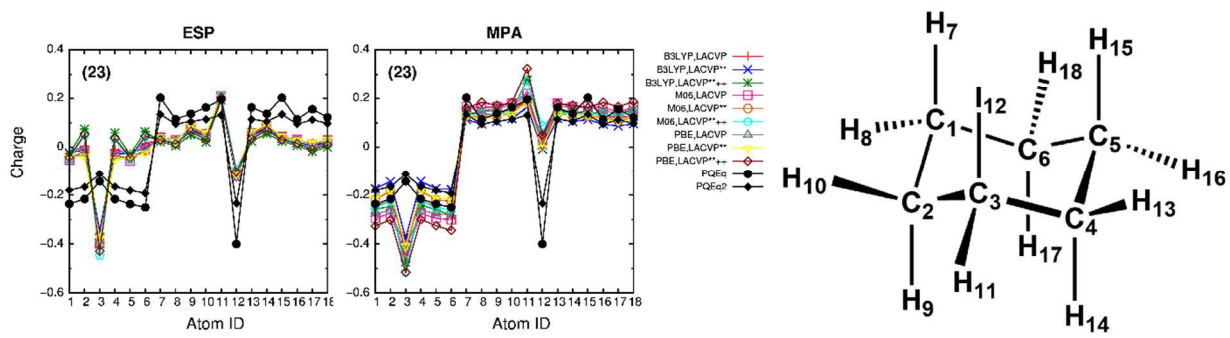
F2
Br1
F4
F5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PQEq2
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H15
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C6
C5
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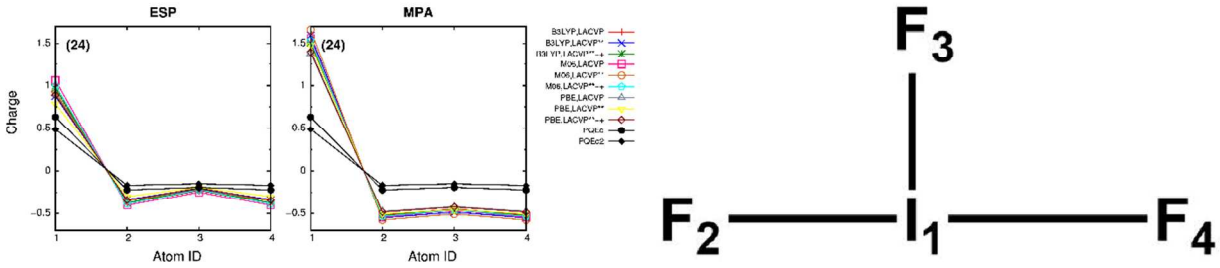
H10
C2
C3
C4
H13
H17
H11
H9
H14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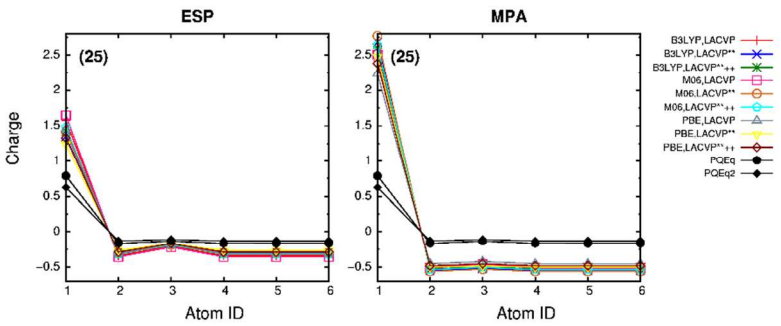
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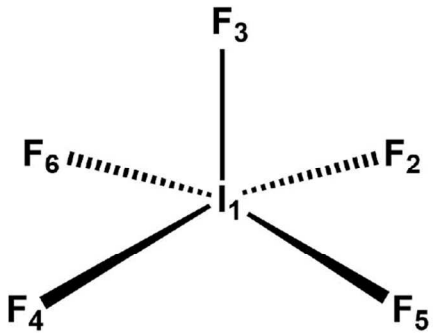
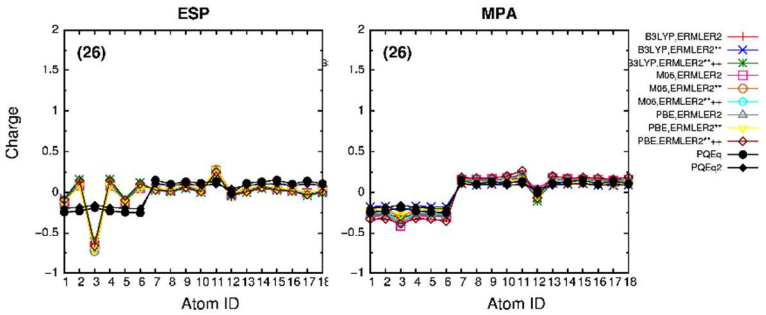
M06,LACVP**++
PBE,LACVP
PBE,LACVP**
PBE,LACVP**++
PQEq
PQEq2


F3
F6
F2
I1
F4
F5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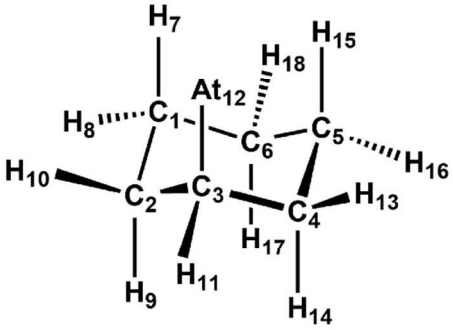
M06,ERMLER2**
M06,ERMLER2**++
PBE,ERMLER2
PBE,ERMLER2**
PBE,ERMLER2**++
PQEq
PQEq2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H18
At12
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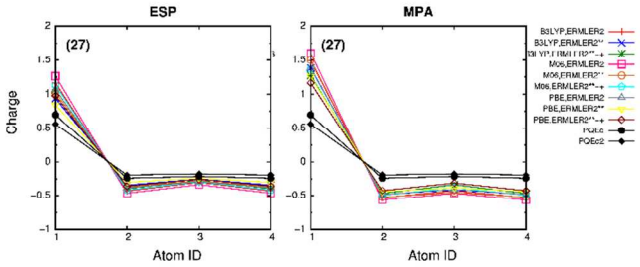
C1
C6
C5
H16
H10
C2
C3
C4
H13
H17
H11
H9
H14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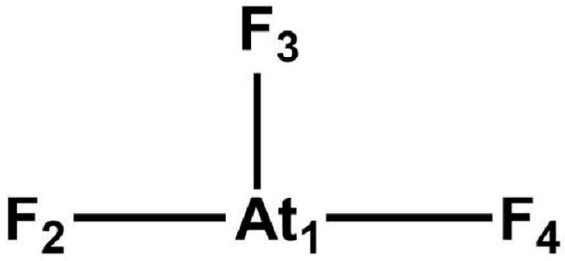
PBE,ERMLER2
PBE,ERMLER2**
PQEq2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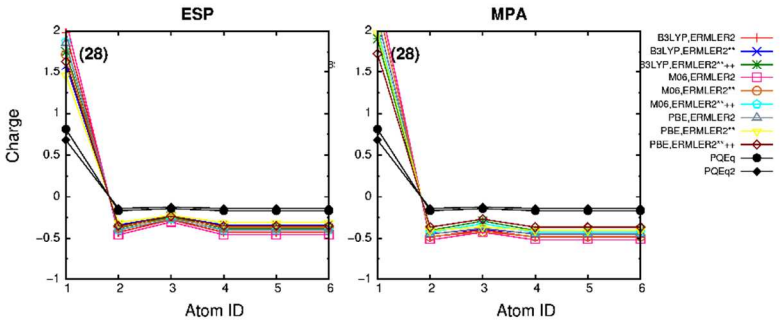
F2
At1
F4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M06,ERMLER2
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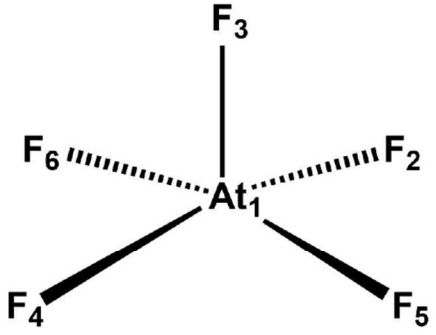
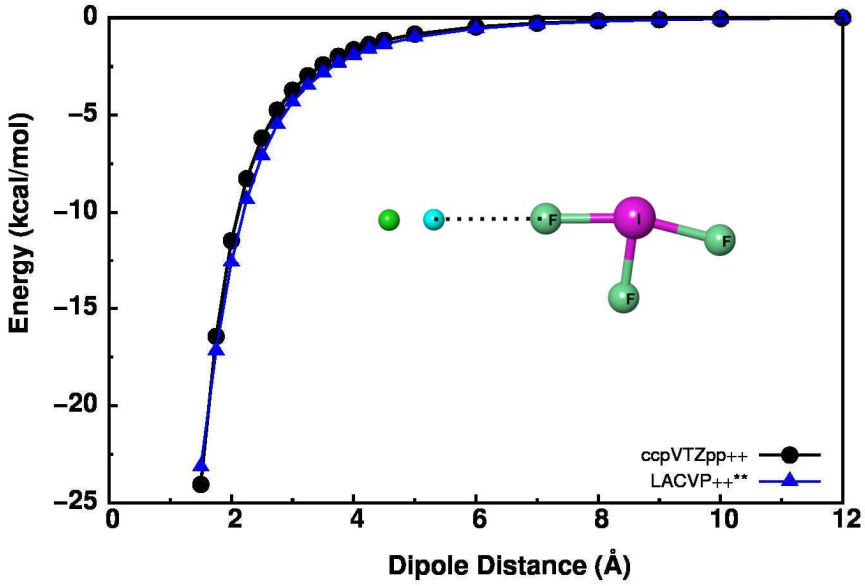
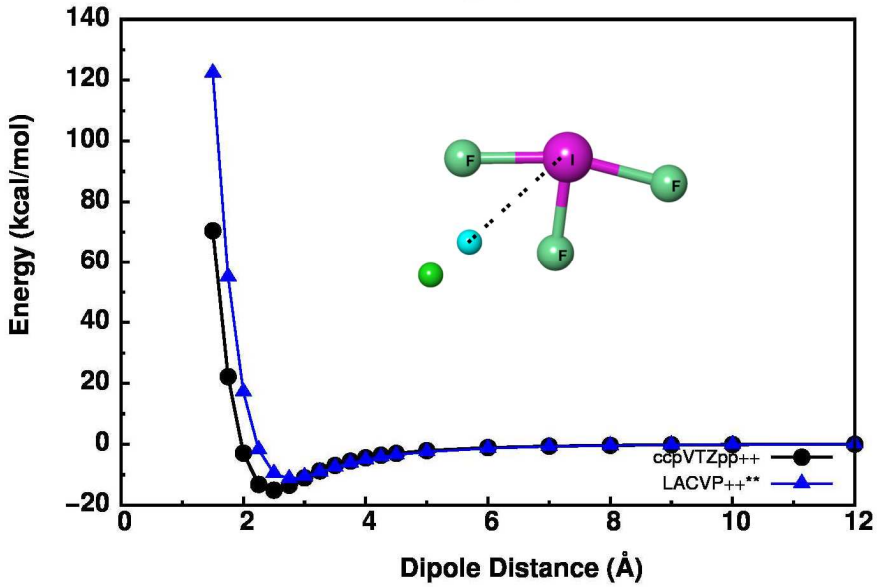
PBE,ERMLER2
PBE,ERMLER2**
PQEq
PQEq2


F3
F6
F2
At1
F4
F5

4. Test of LACVP Basis Set for Iodine

Figure S3: A comparison of the dipole electrostatic interaction curves generated using B3LYP and either LACVP++**[1] or ccpVTZpp++[4-5]. Two different directions are selected for the scans.The software used to calculate the QM energy curves, Jaguar, does not include iodine in the LACVP basis set, but automatically switches to a non-core-valence basis set. This basis set is compared against the correlation-consistent polarized valence triple-zeta basis set that includes effective core potentials for the case of iodine trifluoride. The small difference between the energy curves is acceptable.





5. Molecular Structures of Training Set

Table S2: The geometries of the 28 molecular structures used in the training set. The files are each listed in XYZ file format. The structures were determined by choosing cyclohexane and replacing carbons or hydrogens with elements of interest, or by choosing interhalogen compounds. The structures geometries were then optimized using the B3LYP DFT functional with either the LACVP or ERMLER2 basis sets.

18

156.GeCYC

C	-0.20112	0.36592	0.38095
C	-1.59678	0.49118	-0.26719
Ge	-2.94348	1.05028	1.07704
C	-2.4485	-0.00688	2.68041
C	-0.91472	-0.0515	2.8505
C	-0.14806	-0.56095	1.61275
H	0.15937	1.36285	0.67481

H	0.51297	-0.00291	-0.36833
H	-1.90374	-0.48	-0.67727
H	-1.57115	1.19236	-1.10895
H	-4.38861	0.7762	0.61344
H	-2.79996	2.56	1.37366
H	-2.92603	0.4003	3.57879
H	-2.83735	-1.0258	2.55309
H	-0.54311	0.95176	3.10646
H	-0.66509	-0.69207	3.70767
H	-0.52936	-1.55527	1.33452
H	0.90363	-0.70474	1.89234

18
159.3GeCYC

Ge	-0.08102	0.46033	0.04515
C	-1.99881	0.54497	-0.44361
Ge	-3.20174	1.13332	1.01616
C	-2.88557	0.02826	2.62967
Ge	-0.9946	-0.07329	3.21037
C	0.14314	-0.62632	1.68613
H	0.43844	1.88931	0.30962
H	0.73945	-0.1465	-1.11385
H	-2.31673	-0.45081	-0.77584
H	-2.12169	1.21369	-1.30306
H	-4.67616	1.01831	0.57182
H	-2.90884	2.61145	1.34913
H	-3.49511	0.41467	3.4544
H	-3.24289	-0.9891	2.42875
H	-0.54103	1.31687	3.7036
H	-0.84649	-1.07414	4.37698
H	-0.08377	-1.67189	1.44461
H	1.19477	-0.59937	1.99339

18
162.6GeCYC

Ge	0.26482	0.57224	-0.24234
Ge	-2.12837	0.63583	-0.92402
Ge	-3.57659	1.39884	0.95125
Ge	-3.25511	-0.01635	2.97357
Ge	-0.86207	-0.09861	3.65373
Ge	0.59162	-0.84635	1.77678
H	0.72242	2.00668	0.08302

H	1.13241	0.04745	-1.40207
H	-2.56168	-0.78321	-1.33775
H	-2.30745	1.56241	-2.14153
H	-5.05572	1.37745	0.52155
H	-3.20312	2.85178	1.30086
H	-4.11397	0.51926	4.1349
H	-3.72676	-1.44728	2.65295
H	-0.42416	1.3141	4.08424
H	-0.68922	-1.03895	4.86164
H	0.22876	-2.30051	1.42107
H	2.0697	-0.81681	2.20968

18
164.SnCYC

C	-0.06851	0.28544	0.39842
C	-1.42263	0.46454	-0.32245
Sn	-2.95185	1.05913	1.0756
C	-2.32617	-0.0602	2.80841
C	-0.78566	-0.13387	2.88352
C	-0.08306	-0.66519	1.61522
H	0.30995	1.26542	0.72558
H	0.6708	-0.0914	-0.32295
H	-1.73165	-0.48608	-0.77614
H	-1.33047	1.18595	-1.14166
H	-4.53043	0.64975	0.55519
H	-2.89889	2.74653	1.37175
H	-2.73723	0.36908	3.72863
H	-2.74374	-1.07179	2.72172
H	-0.37759	0.86071	3.11774
H	-0.50114	-0.77713	3.72864
H	-0.53629	-1.62475	1.32255
H	0.95856	-0.89137	1.87764

18
167.3SnCYC

Sn	0.0482	0.45207	-0.0904
C	-2.03985	0.57391	-0.59408
Sn	-3.37516	1.19071	0.97594
C	-3.00095	0.0156	2.73887
Sn	-0.95381	-0.13369	3.38317
C	0.28532	-0.69277	1.71541
H	0.65708	2.03221	0.16471

H	0.92719	-0.27011	-1.37274
H	-2.3636	-0.41183	-0.9497
H	-2.15556	1.25997	-1.44111
H	-5.00457	1.00787	0.47597
H	-3.0962	2.84185	1.33426
H	-3.59675	0.42495	3.56297
H	-3.37845	-0.99857	2.56036
H	-0.44163	1.38815	3.97836
H	-0.8086	-1.28899	4.64123
H	0.08785	-1.74604	1.48185
H	1.33483	-0.6383	2.02716

18

169.6SnCYC

Sn	0.51566	0.60288	-0.47279
Sn	-2.2141	0.69515	-1.24926
Sn	-3.87304	1.55652	0.88825
Sn	-3.50723	-0.04948	3.20127
Sn	-0.77887	-0.16314	3.97975
Sn	0.89072	-1.00015	1.84078
H	1.03218	2.19424	-0.11871
H	1.4795	0.01911	-1.75873
H	-2.69949	-0.87781	-1.71263
H	-2.41091	1.71882	-2.60446
H	-5.51434	1.54061	0.40953
H	-3.4614	3.17024	1.27677
H	-4.46442	0.54062	4.48935
H	-4.03678	-1.63642	2.84638
H	-0.28983	1.40043	4.47036
H	-0.58989	-1.20924	5.31899
H	0.49929	-2.61811	1.44906
H	2.53032	-0.96595	2.32459

18

171.PbCYC

C	0.01468	0.23908	0.4135
C	-1.32037	0.42762	-0.3315
Pb	-2.90629	1.03634	1.08499
C	-2.2409	-0.10631	2.85813
C	-0.70322	-0.18067	2.90146
C	-0.02075	-0.71885	1.62464
H	0.39257	1.21555	0.75096

H	0.76444	-0.13731	-0.29834
H	-1.64246	-0.51568	-0.78854
H	-1.2236	1.16344	-1.13601
H	-4.5063	0.5963	0.55513
H	-2.87577	2.75556	1.37922
H	-2.64153	0.34093	3.7733
H	-2.67234	-1.11063	2.76962
H	-0.28947	0.81352	3.12622
H	-0.40526	-0.82187	3.74445
H	-0.49585	-1.66639	1.32773
H	1.01639	-0.9703	1.88148

18
174.3PbCYC

Pb	0.08099	0.44808	-0.12523
C	-2.06033	0.56004	-0.65032
Pb	-3.42003	1.20339	0.96548
C	-3.04667	-0.01311	2.76946
Pb	-0.94369	-0.14912	3.42677
C	0.32451	-0.74038	1.71902
H	0.69405	2.05624	0.14325
H	0.9767	-0.28476	-1.43286
H	-2.37945	-0.43145	-0.98839
H	-2.17517	1.24797	-1.49402
H	-5.07973	1.02039	0.45518
H	-3.12367	2.87983	1.33372
H	-3.63961	0.39859	3.59246
H	-3.41056	-1.02796	2.57767
H	-0.42644	1.40581	4.01702
H	-0.79223	-1.32164	4.71153
H	0.10826	-1.78722	1.48132
H	1.37243	-0.68375	2.0305

18
176.6PbCYC

Pb	0.5707	0.58263	-0.52784
Pb	-2.22185	0.71518	-1.32326
Pb	-3.9397	1.58053	0.85556
Pb	-3.56845	-0.02223	3.25212
Pb	-0.78116	-0.21449	4.05531
Pb	0.97279	-1.0025	1.87533
H	1.12128	2.21468	-0.23833

H	1.52755	-0.03879	-1.85134
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H	-5.62293	1.53783	0.38781
H	-3.57636	3.24171	1.25358
H	-4.50961	0.61538	4.57945
H	-4.1549	-1.64088	2.95836
H	-0.24174	1.33759	4.64668
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H	2.64832	-0.89714	2.36089

18
178.AsOCYC

C	0.0021	1.31341	0.17496
C	-1.49686	1.29	-0.17785
C	-2.42001	1.83495	0.92808
C	-2.43589	0.98625	2.21228
As	-0.62897	0.78006	2.965
C	0.39322	0.3769	1.33221
H	0.29825	2.34428	0.41621
H	0.5869	1.03121	-0.70978
H	-1.7961	0.26196	-0.42843
H	-1.65083	1.8858	-1.08561
H	-3.44611	1.89908	0.54419
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H	-3.07985	1.42315	2.98162
H	-2.80395	-0.02667	2.01436
H	-0.22929	2.22189	3.25213
O	-0.45021	-0.24612	4.24911
H	0.1796	-0.6693	1.08622
H	1.45928	0.44532	1.56956

18
180.SbOCYC

C	-0.30583	0.38116	0.38938
C	-1.67143	0.58269	-0.2964
Sb	-3.13078	1.32199	1.10645
C	-2.55626	0.06887	2.76287
C	-1.02212	-0.03587	2.86548
C	-0.31381	-0.57017	1.60359
H	0.09686	1.35539	0.69832

H	0.39524	-0.01124	-0.35917
H	-2.05379	-0.36441	-0.69679
H	-1.59987	1.29173	-1.12659
H	-4.61503	0.68716	0.57049
O	-3.14317	3.12309	1.40518
H	-2.99008	0.48428	3.67736
H	-3.00728	-0.9173	2.59643
H	-0.60362	0.94631	3.12394
H	-0.78268	-0.69724	3.70873
H	-0.76168	-1.53216	1.31211
H	0.72797	-0.78812	1.86831

18

182.BiOCYC

C	-0.27835	0.41101	0.35781
C	-1.61732	0.61348	-0.36967
Bi	-3.15703	1.37486	1.06184
C	-2.53224	0.09438	2.78423
C	-0.99885	0.00235	2.84144
C	-0.31263	-0.54309	1.57081
H	0.11836	1.38435	0.67696
H	0.44329	0.01895	-0.37267
H	-2.00729	-0.32782	-0.77359
H	-1.53607	1.33658	-1.18564
O	-3.19538	3.2567	1.36266
H	-2.95117	0.53434	3.69321
H	-2.99304	-0.88744	2.6263
H	-0.57929	0.98878	3.08142
H	-0.73406	-0.64877	3.68642
H	-0.78333	-1.49355	1.27784
H	0.7243	-0.7875	1.83132
H	-4.68723	0.68815	0.50343

12

184.AsAcid

As	-0.50153	0.82652	1.415
C	-1.57995	2.08067	2.43965
C	-1.70184	-0.19624	0.27499
O	0.24879	1.93433	0.20941
O	0.59917	-0.04247	2.2657
H	-0.90938	2.69826	3.03997
H	-2.15044	2.71235	1.75535

H	-2.25517	1.52974	3.09839
H	-1.09829	-0.84364	-0.36385
H	-2.36148	-0.80839	0.89426
H	-2.28875	0.48772	-0.34185
H	1.21447	1.84933	0.23444

17
187.SeOCYC

C	-0.54761	1.13631	0.32914
C	-1.94764	1.06904	-0.27055
Se	-3.29874	1.89455	1.0029
C	-2.75897	0.63047	2.49971
C	-1.26452	0.74904	2.77672
C	-0.37611	0.29354	1.60545
H	-0.31505	2.18631	0.54633
H	0.16756	0.80067	-0.43365
H	-2.29422	0.04644	-0.45678
H	-2.03572	1.65229	-1.19024
H	-3.36694	0.93343	3.35548
H	-3.06505	-0.37019	2.17501
H	-1.04115	1.79428	3.02443
H	-1.03381	0.1518	3.66896
H	-0.5803	-0.76384	1.37827
H	0.6727	0.34537	1.92091
O	-2.53875	3.35282	1.45671

18
188.SeOOCYC

C	-0.45919	1.21039	0.35235
C	-1.86017	1.13234	-0.25808
Se	-3.2099	1.75357	1.06795
C	-2.62472	0.67392	2.63593
C	-1.11347	0.81888	2.82837
C	-0.27368	0.35687	1.62186
H	-0.22215	2.25839	0.57126
H	0.25167	0.88097	-0.41607
H	-2.1701	0.11494	-0.51299
H	-1.99142	1.78349	-1.12516
H	-3.20628	1.05573	3.47796
H	-2.94019	-0.3473	2.40449
H	-0.88166	1.86444	3.06382
H	-0.83809	0.22915	3.71197

H	-0.50309	-0.69432	1.395
H	0.78412	0.38752	1.90629
O	-2.8699	3.33631	1.41101
O	-4.71498	1.27015	0.5911

17
190.TeOCYC

C	-0.40232	1.06009	0.35473
C	-1.78531	0.9914	-0.29663
Te	-3.29344	1.8841	1.00994
C	-2.62833	0.53572	2.59683
C	-1.12056	0.6725	2.8191
C	-0.25561	0.21188	1.63149
H	-0.16913	2.10816	0.58283
H	0.33921	0.72661	-0.38415
H	-2.1083	-0.03711	-0.49747
H	-1.82124	1.55498	-1.23337
H	-3.19687	0.81163	3.4896
H	-2.92231	-0.47729	2.29707
H	-0.89039	1.71947	3.05526
H	-0.85243	0.08388	3.70721
H	-0.48223	-0.84008	1.40002
H	0.79595	0.23834	1.94219
O	-2.46582	3.44047	1.49705

18
191.TeOOCYC

C	-0.3058	1.18086	0.37141
C	-1.6866	1.1268	-0.29989
Te	-3.21303	1.77159	1.06478
C	-2.47928	0.65604	2.74788
C	-0.95396	0.7952	2.86266
C	-0.15911	0.30959	1.63449
H	-0.05779	2.22219	0.61257
H	0.42979	0.85444	-0.37501
H	-1.97297	0.11229	-0.59589
H	-1.75208	1.78019	-1.17383
H	-3.0019	1.03775	3.62882
H	-2.79786	-0.37603	2.56838
H	-0.69782	1.84057	3.07622
H	-0.64196	0.21642	3.74161
H	-0.43871	-0.72801	1.40118

H	0.90225	0.28648	1.90717
O	-2.95256	3.51508	1.3988
O	-4.80797	1.13833	0.5485

17
193.PoOCYC

C	-0.26865	0.99686	0.37983
C	-1.62479	0.93956	-0.32545
Po	-3.26072	1.91392	1.02226
C	-2.5047	0.47882	2.69892
C	-0.98988	0.61936	2.85867
C	-0.15784	0.13788	1.65434
H	-0.03182	2.04115	0.62235
H	0.49912	0.66298	-0.33355
H	-1.95368	-0.08588	-0.53222
H	-1.62953	1.50948	-1.25895
H	-3.04433	0.76931	3.60483
H	-2.80987	-0.53442	2.4115
H	-0.74567	1.66773	3.07471
H	-0.68723	0.042	3.74464
H	-0.42514	-0.90349	1.41796
H	0.89601	0.1198	1.9582
O	-2.33582	3.57775	1.54564

20
195.PoOOCYC

C	-0.18657	1.17729	0.39317
C	-1.52514	1.10757	-0.34798
Po	-3.23149	1.79311	1.06265
C	-2.35239	0.64085	2.87093
C	-0.83066	0.8113	2.90136
C	-0.06941	0.30335	1.65922
H	0.04396	2.22063	0.64409
H	0.58764	0.86267	-0.32182
H	-1.81569	0.09302	-0.63791
H	-1.5725	1.76899	-1.21619
H	-2.85004	1.04832	3.754
H	-2.6768	-0.39121	2.70529
H	-0.57941	1.8645	3.08099
H	-0.4683	0.26179	3.78244
H	-0.38089	-0.72571	1.42903
H	0.99276	0.24532	1.92369

O	-2.98448	3.71021	1.40104
O	-4.92916	0.97986	0.51293
O	-4.92916	0.97986	0.51293
O	-4.92916	0.97986	0.51293

18
197.BrCYC

C	-0.57494	0.39924	0.38915
C	-2.05208	0.47968	-0.02574
C	-2.9774	0.88571	1.11784
C	-2.75008	0.07152	2.38842
C	-1.27196	-0.00817	2.80004
C	-0.38646	-0.48178	1.63539
H	-0.20424	1.41119	0.5943
H	0.01672	0.00894	-0.44753
H	-2.39157	-0.51795	-0.34874
H	-2.18759	1.14964	-0.88051
H	-4.02345	0.86581	0.81192
Br	-2.73207	2.90073	1.52919
H	-3.36822	0.45933	3.20414
H	-3.11881	-0.9432	2.16666
H	-0.93941	0.98177	3.13616
H	-1.16939	-0.68422	3.65729
H	-0.63987	-1.52327	1.38618
H	0.6671	-0.48199	1.93994

4
199.BrF3

Br	0	0	-0.29611
F	0	1.88339	-0.13574
F	0	0	1.5015
F	0	-1.88339	-0.13574

6
201.BrF5

Br	0	0	-0.27394
F	1.83693	0	-0.09032
F	0	1.83693	-0.09032
F	-1.83693	0	-0.09032
F	0	-1.83693	-0.09032
F	0	0	1.49922

18
203.ICYC

C	-0.5192	0.37199	0.39998
C	-1.99665	0.46202	-0.01065
C	-2.9185	0.88078	1.13424
C	-2.69342	0.05456	2.40021
C	-1.21636	-0.03578	2.81261
C	-0.332	-0.50866	1.6467
H	-0.13896	1.38149	0.60153
H	0.06746	-0.02379	-0.43769
H	-2.34178	-0.53733	-0.32415
H	-2.12748	1.1223	-0.87358
H	-3.96447	0.85736	0.82796
I	-2.68151	3.07835	1.57359
H	-3.31103	0.43026	3.22189
H	-3.06183	-0.95841	2.1673
H	-0.87711	0.94978	3.15596
H	-1.11823	-0.7173	3.66609
H	-0.58692	-1.54953	1.39708
H	0.72173	-0.5106	1.95077

4
204.IF3

I	0	0	-0.25036
F	0	1.95185	0.01619
F	0	0	1.63998
F	0	-1.95185	0.01619

6
206.IF5

I	0	0	0.24814
F	1.88888	0	-0.01604
F	0	0	-1.59338
F	-1.88888	0	-0.01604
F	0	1.88888	-0.01604
F	0	-1.88888	-0.01604

18
208.AtCYC

C	-0.46728	0.31033	0.40356
C	-1.94477	0.40303	-0.00787
C	-2.86791	0.81634	1.13719

C	-2.64248	-0.00493	2.40541
C	-1.16486	-0.09707	2.81651
C	-0.28275	-0.57189	1.64964
H	-0.08526	1.31902	0.60751
H	0.12019	-0.08499	-0.43372
H	-2.28606	-0.59658	-0.3279
H	-2.07334	1.06416	-0.87062
H	-3.91465	0.80294	0.83199
At	-2.64363	3.14782	1.59659
H	-3.25827	0.37121	3.22839
H	-3.01077	-1.02057	2.1797
H	-0.82308	0.88861	3.15804
H	-1.06572	-0.7775	3.67069
H	-0.54238	-1.61132	1.39913
H	0.77107	-0.5789	1.95316

4
209.AtF3

At	0	0	-0.14817
F	0	2.08743	-0.11899
F	0	0	1.87566
F	0	-2.08743	-0.11899

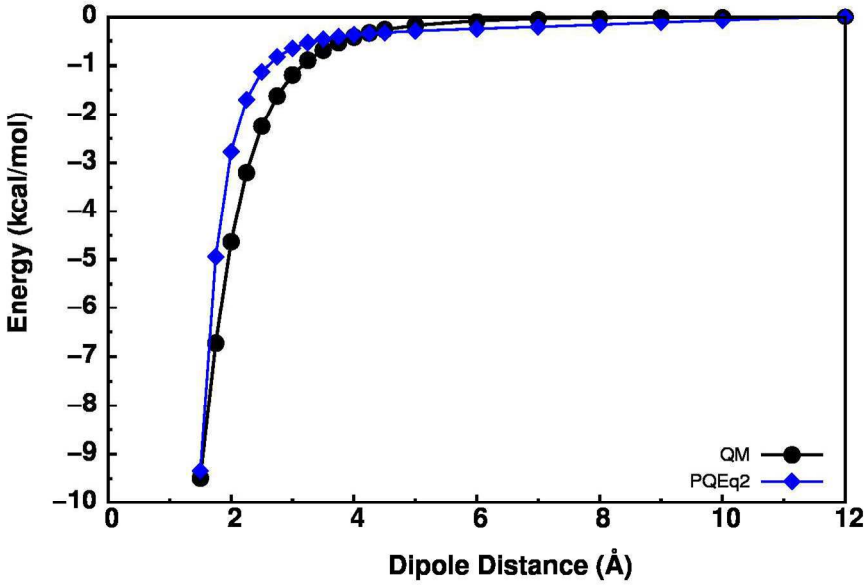
6
211.AtF5

At	0	0	0.15785
F	2.03483	0	0.01976
F	0	0	-1.82375
F	-2.03483	0	0.01976
F	0	2.03483	0.01976
F	0	-2.03483	0.01976

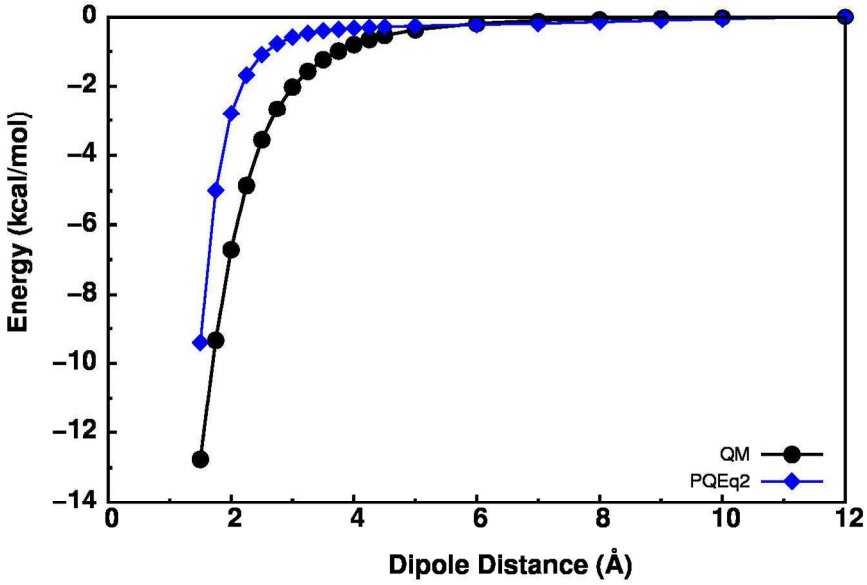
6. Dipole Scans of Other Oxidation States

Figure S4: A comparison between QM (LACVP**++ and B3LYP) with PQEq2 via the electrostatic interaction dipole energies, for As(III) in $HAsC_5H_{10}$, Sb(III) in $HSbC_5H_{10}$, and Bi(III) in $HBiC_5H_{10}$. Each dipole scan was directed along the H-As (or respective) bond.

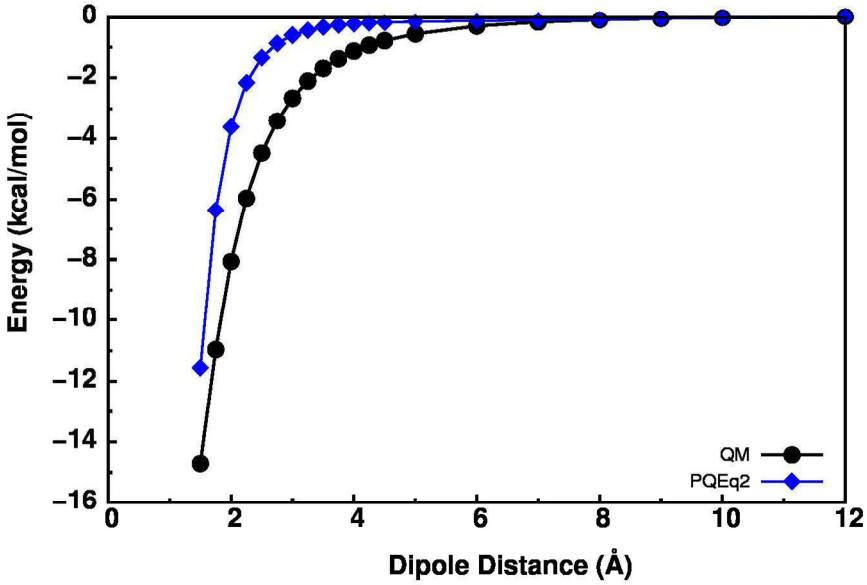
a)


Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq2

b)


Energy (kcal/mol)
Dipole Distance (Å)
QM
PQEq2

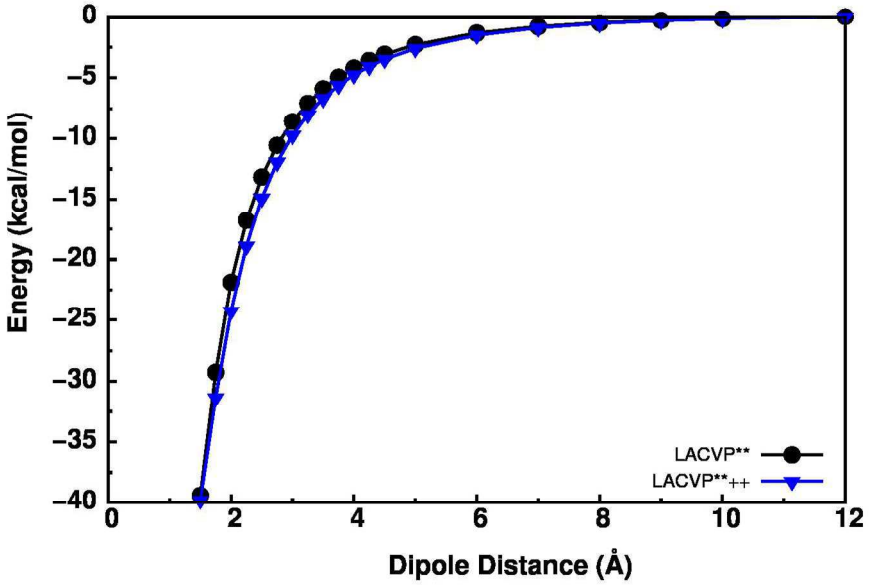
c)



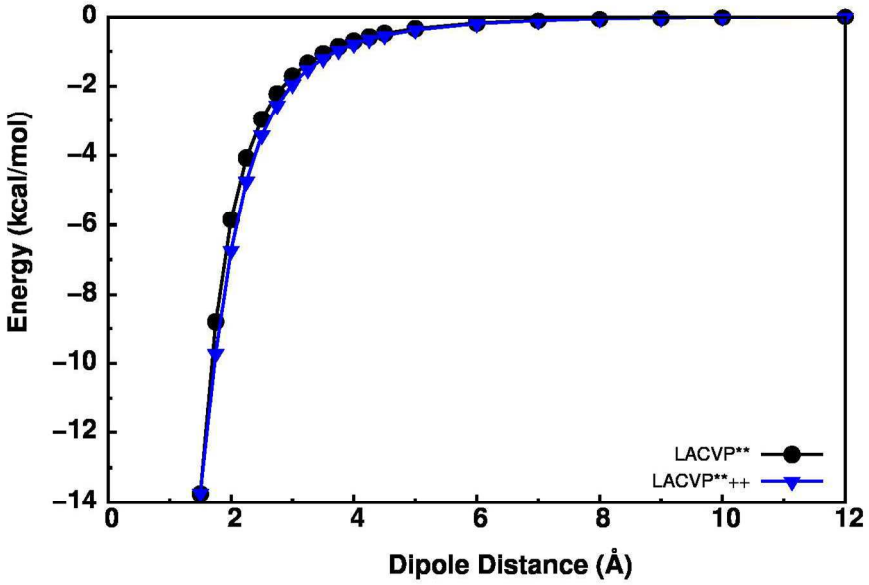
7. Effects of Functionals on Electrostatic Interaction Dipole Scans

Figure S5: A comparison between (a, b) diffuse functionals for B3LYP/LACVP** scanning dipoles towards $OSeC_5H_{10}$ (along O-Se bond) and BrF_5 (along Br-F bond), and a comparison between (c) different DFT functionals (B3LYP, M06, and HFS) using LACVP**++ basis set and $OAsC_5H_{10}$ (along O-As bond).

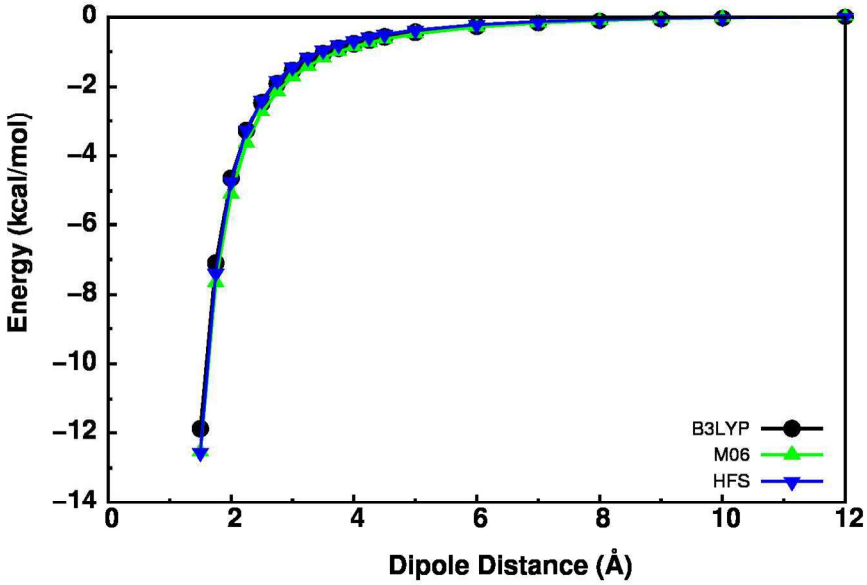
a)


Energy (kcal/mol)
0
−5
−10
−15
−20
−25
−30
−35
−40
0
2
4
6
8
10
12
Dipole Distance (Å)
LACVP**
LACVP**++

b)

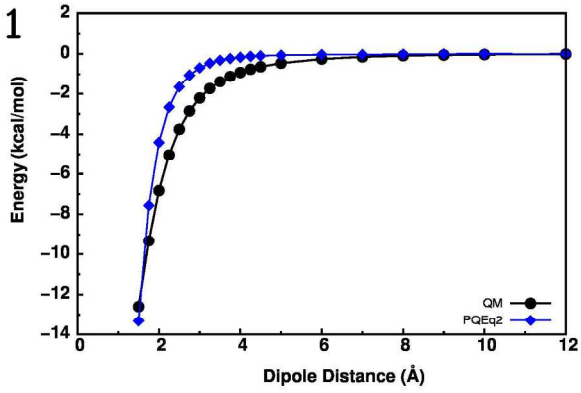

Energy (kcal/mol)
0
−2
−4
−6
−8
−10
−12
−14
0
2
4
6
8
10
12
Dipole Distance (Å)
LACVP**
LACVP**++

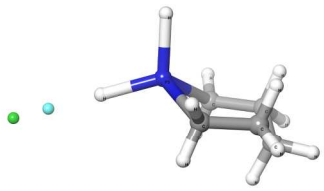
c)

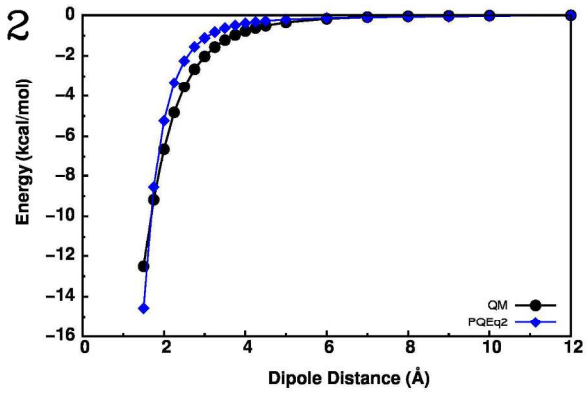


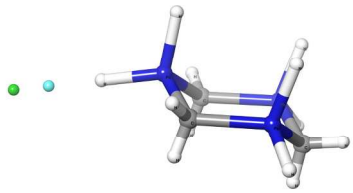
8. Effect of Direction on Electrostatic Interaction Dipole Scans

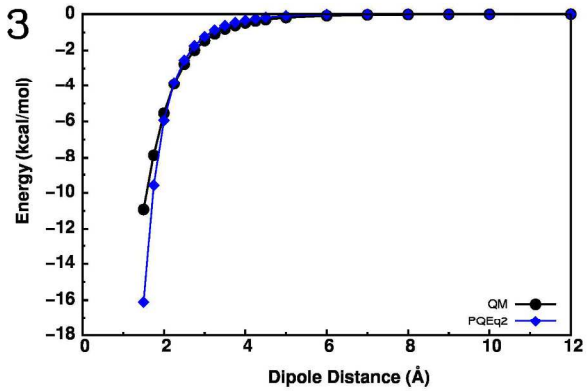
Figure S6: The effect of direction of dipole scans for Pb containing cyclohexane based structures. When the dipole is scanned along the equatorial hydrogen bond the Pb atoms are polarized, rather than scanning along the axial hydrogen bond, where the hydrogen bonds are polarized.

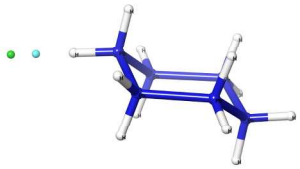












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